Supporting Information

The fcc structure isomerization in gold nanoclusters

Shengli Zhuang[+, a, b], Lingwen Liao[+, a], Man-Bo Li[a], Chuanhao Yao[a], Yan Zhao[a, b], Hongwei Dong[a, b], Jin Li[c], Haiteng Deng[d], Lingling Li[e], and Zhikun Wu*[, a]

[a] Key Laboratory of Materials Physics, Anhui Key Laboratory of Nanomaterials and Nanotechnology, CAS Center for Excellence in Nanoscience, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei, Anhui 230031, China

E-mail: zkwu@issp.ac.cn

[b] Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026, China

[c] Tsinghua University-Peking University Joint Center for Life Sciences, School of Life Sciences, Tsinghua University, Beijing 100084, China

[d] MOE Key Laboratory of Bioinformatics, School of Life Sciences, Tsinghua University, Beijing 100084, China

[e] Instrumental Analysis Center, Shanghai Jiaotong University, S hanghai 200240, China

[+] S. Zhuang and L. Liao contributed equally to this work.

1. Experimental

1.1 Chemicals.

All chemicals are commercially available and used as received. Tetrachloroauric(III) acid ($HAuCl_4 \cdot 4H_2O$, >99.99% metals basis, Sigma-Aldrich), tetraoctylammonium bromide (TOAB, ≥98%, Aladdin), phenylethylthiol (PET, 99%, Sigma-Aldrich), 4-tert-butylbenzenethiol (TBBTH, 97%, Sigma-Aldrich), sodium borohydride ($NaBH_4$, Sigma-Aldrich). Solvents: tetrahydrofuran (THF, 99.0%), ethanol (AR, 99.7%), methanol (CH_3OH, 99.5%), toluene (C_7H_8, 99.5%), dichloromethane (CH_2Cl_2, 99.0%), petroleum ether (AR), hydrochloric acid (AR, 36.0%~38.0%), nitric acid (AR, 65%~68%) and acetic acid (AR, 99.50%) were purchased from Sinopharm chemical reagent co., ltd. The water used in all experiments was ultrapure (resistivity 18.2 MΩ cm), produced by a Milli-Q NANO pure water system.

1.2 Synthesis of $Au_{52}(PET)_{32}$.

Tetraoctylammonium bromide (TOAB, 200 mg) was dissolved in 15 mL of THF in a tri-neck flask, and then $HAuCl_4 \cdot 4H_2O$ (100 mg, 0.243 mmol) and 75 μL of nitric acid (4.6 equivs./mol of Au) dissolved in 75 μL of water were added into the solution. After the solution was stirred for 15 min, 400 μL of phenylethylthiol (12.2 equivs./mol of Au) was added. The solution was kept under constant stirring (900 rpm) until the colour of the solution changed from deep red to colorless over a duration of 3 h, and then a freshly made cold aqueous solution of $NaBH_4$ (130 mg, 14.1 equivs./mol of Au) was added at one time. The growth of gold nanoclusters was allowed to proceed for overnight (~15 h). After removal of the indissolvable, the solution was concentrated

and cold water was added, the precipitates were collected and thoroughly washed with methanol, then the $Au_{52}(PET)_{32}$ nanoclusters were isolated from the crude by PTLC (CH_2Cl_2–petroleum ether as developing solvent) in a yield of ~0.5% (on basis of gold atoms). It should be noted that the whole process (including the reaction, post-treatment and isolation by PTLC) was facilely conducted at room temperature without the avoidance of light and air.

Syntheses of $Au_{52}(PET)_{32}$ nanoclusters with the other two acids are similar to the above synthesis method except that 75 μL nitric acid dissolved in 75 μL water is replaced by 150 μL hydrochloric acid (7.4 equivs./mol of Au) dissolved in 240 μL water or 150 μL acetic acid (10.8 equivs./mol of Au) dissolved in 150 μL water.

Synthesis of $Au_{52}(TBB)_{32}$ nanocluster was referred to the previous work[1].

1.3 Characterization.

Electrospray ionization (ESI) mass spectra were collected on a Waters Q-TOF mass spectrometer using a Z-spray source. The source temperature was kept at 70 °C. The spray voltage was adjusted to 2.20 kV and the cone voltage was kept at 60 V. The sample was prepared by dissolving the nanoclusters in toluene (~0.5 mg/mL) and then diluted (2:1 v/v) with methanol solution which contains 50 mM CsOAc. The prepared sample was directly infused into the chamber at 5 μL/min. UV2600 spectrophotometer was employed to record all the UV/vis/NIR absorption spectra in the range of 190-900 nm at room temperature in dichloromethane. The single-crystal X-ray diffraction data were collected on a Bruker D8 VENTURE CMOS photon 100 diffractometer with helios mx multilayer monochrmator Cu Kα radiation (λ = 1.54178 Å).

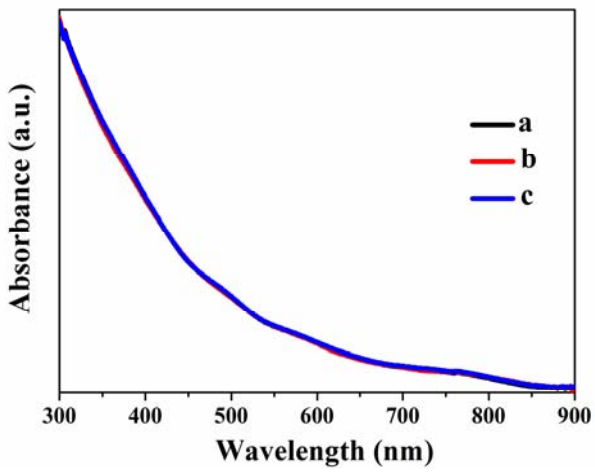

Figure S1. UV/vis/NIR optical spectrum of the major product when various acid was used: a) nitric acid, b) hydrochloric acid, and c) acetic acid.

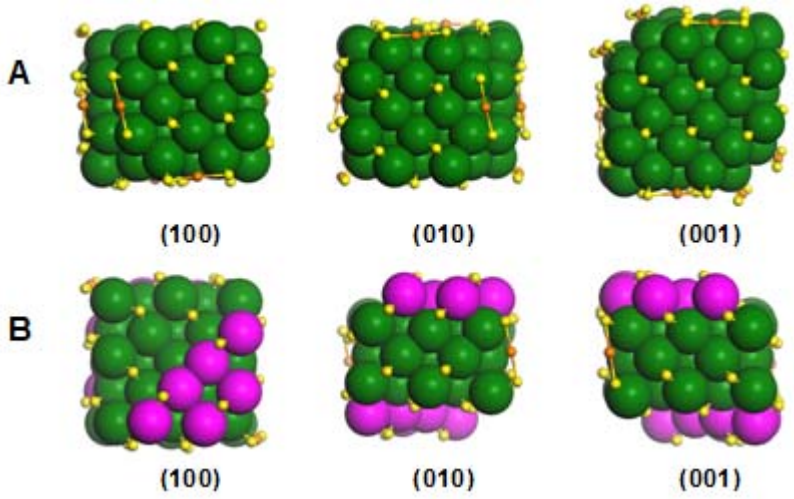

Figure S2. Binding and patterning structures of thiolates on the {100} facets: (A) $Au_{92}(TBBT)_{44}$; (B) $Au_{52}(PET)_{32}$.

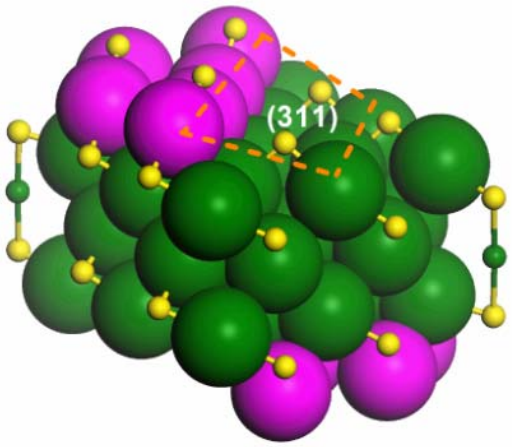

Figure S3. The fragment (311) facets in the $Au_{52}(PET)_{32}$ nanoclusters.

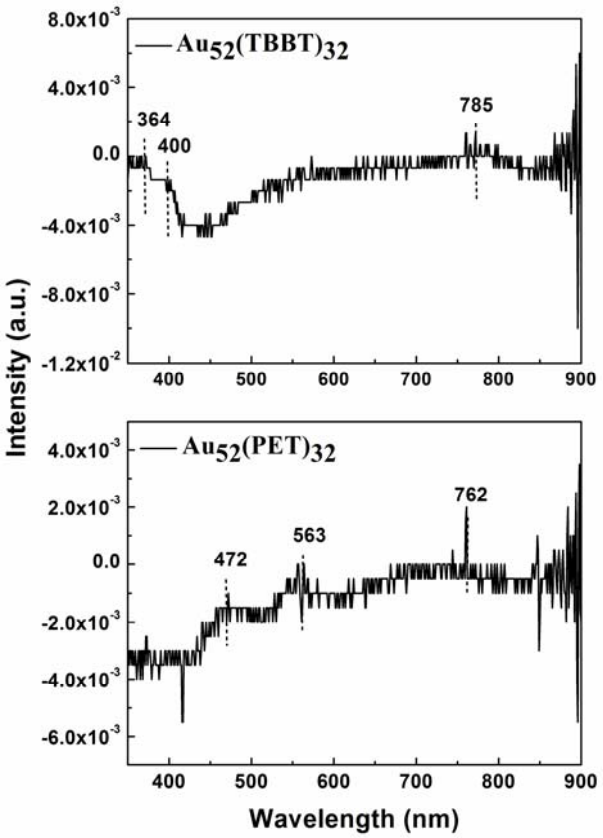

Figure S4. The first derivatives of UV/vis/NIR absorption spectra of $Au_{52}(PET)_{32}$ and $Au_{52}(TBBT)_{32}$.

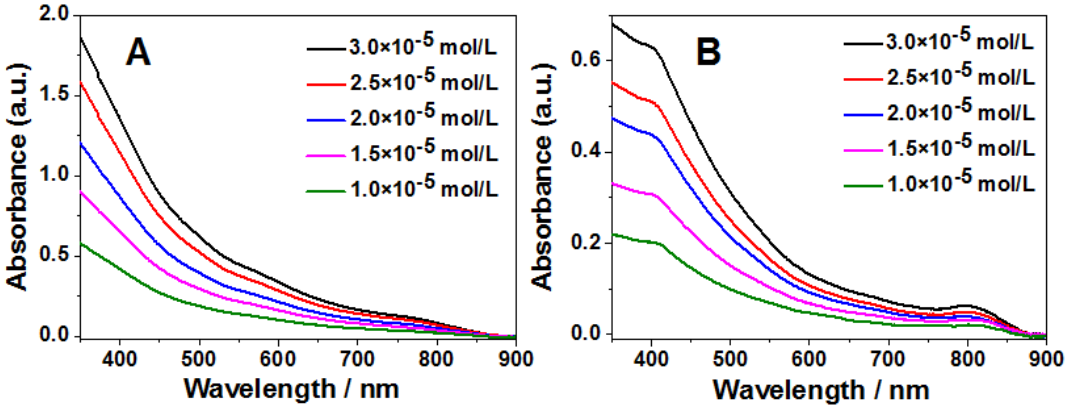

Figure S5. The UV/vis/NIR absorption spectra of the two $Au_{52}(SR)_{32}$ in different concentrations: (A) $Au_{52}(PET)_{32}$; (B) $Au_{52}(TBBT)_{32}$.

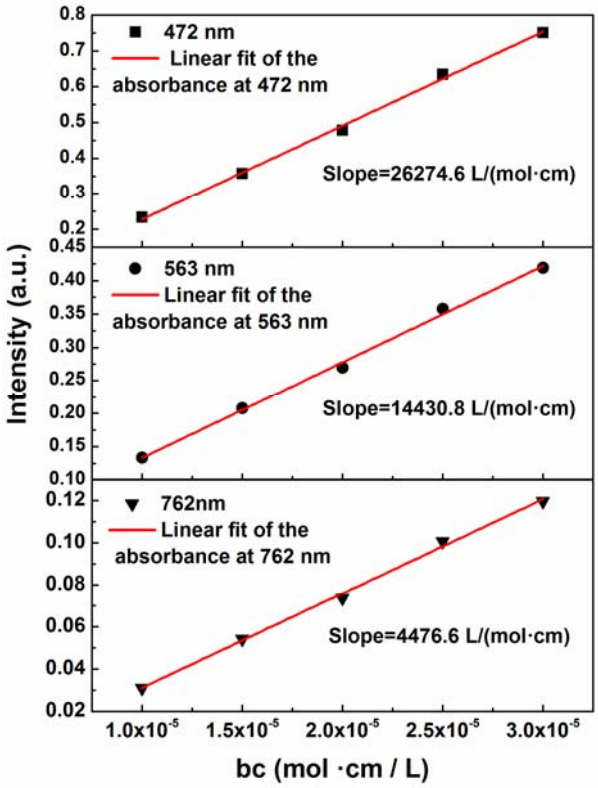

Figure S6. The extinction coefficients of $Au_{52}(PET)_{32}$ at 472, 563 and 762 nm.

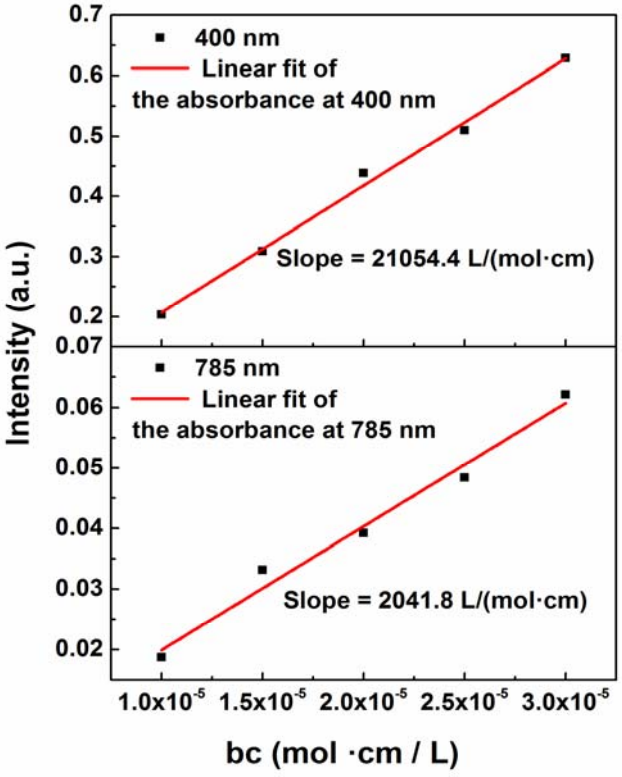

Figure S7. The extinction coefficients of $Au_{52}(TBBT)_{32}$ at 400 and 785 nm.

1.4 Reference

1. C. Zeng, Y. Chen, C. Liu, K. Nobusada, N. L. Rosi and R. Jin, *Sci. Adv.*, 2015, 1, e1500425.

2. Single crystal data of $Au_{52}(PET)_{32}$

Table 1. Crystal data and structure refinement for $Au_{52}(PET)_{32}$.

Identification code $Au_{52}(PET)_{32}$

Empirical formula	$C_{256}\,H_{288}\,Au_{52}\,S_{32}$	
Formula weight	14633.03	
Temperature	173.0 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 19.2220(8) Å	α= 116.588(2)°.
	b = 19.8976(8) Å	β= 95.458(2)°.
	c = 21.4243(9) Å	γ = 95.019(2)°.
Volume	7216.1(5) $Å^3$	
Z	1	
Density (calculated)	3.367 Mg/m^3	
Absorption coefficient	50.734 mm^{-1}	
F(000)	6444	
Crystal size	0.15x 0.13 x 0.12 mm^3	
Theta range for data collection	2.333 to 68.561°.	
Index ranges	-21<=h<=23, -23<=k<=23, -25<=l<=25	
Reflections collected	96113	
Independent reflections	24899 [R(int) = 0.0804]	
Completeness to theta = 67.679°	94.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.1665 and 0.0411	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	24899 / 1747 / 1339	
Goodness-of-fit on F^2	1.458	
Final R indices [I>2sigma(I)]	R1 = 0.1352, wR2 = 0.3636	
R indices (all data)	R1 = 0.1836, wR2 = 0.4084	
Extinction coefficient	n/a	
Largest diff. peak and hole	11.313 and -5.684 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2x10^3$) for $Au_{52}(PET)_{32}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	3992	3605	3405	46(1)
Au(2)	3005	3213	4248	53(1)
Au(3)	4238	2488	3784	57(1)
Au(4)	5121	2838	3036	54(1)
Au(5)	4961	4036	2592	56(1)
Au(6)	3646	4643	2912	60(1)
Au(7)	2750	4245	3640	56(1)
Au(8)	3912	4662	4879	40(1)
Au(9)	4920	5067	4041	41(1)
Au(10)	4547	6219	3446	74(1)
Au(11)	3739	5753	4453	51(1)
Au(12)	2498	5403	5091	60(1)
Au(13)	3899	5741	6403	47(1)
Au(14)	4862	6085	5511	40(1)
Au(15)	5885	6533	4726	50(1)
Au(16)	7013	5749	4374	55(1)
Au(17)	7136	4591	2686	72(1)
Au(18)	6174	2979	1974	74(1)
Au(19)	3168	1862	4531	80(1)
Au(20)	3069	3050	6179	79(1)
Au(21)	4166	4606	6772	57(1)
Au(22)	2939	3196	2303	70(1)
Au(23)	2970	1923	2590	73(1)
Au(24)	4119	2377	1679	82(1)
Au(25)	2189	5580	3299	83(1)
Au(26)	1669	3717	1892	104(1)
S(1)	7921	5306	3706	84(3)
S(2)	6560	3794	1539	115(4)
S(3)	5945	2111	2402	76(3)
S(4)	3697	1316	1804	106(4)
S(5)	4058	1361	3905	110(4)
S(6)	2282	2312	5156	111(4)
S(7)	3809	3760	7207	155(6)
S(8)	2121	2416	3254	80(3)

S(9)	1702	4558	4107	66(2)
S(10)	3082	6433	6101	63(2)
S(11)	3087	6491	4069	77(3)
S(12)	5032	7237	4496	79(3)
S(13)	3984	5374	2330	108(4)
S(14)	4601	3257	1358	115(4)
S(15)	2105	2617	1267	141(5)
S(16)	1219	4808	2557	138(5)
C(1)	8352	5971	3476	93(4)
C(2)	9003	5720	3142	101(4)
C(3)	9357	6135	2782	107(5)
C(8)	9753	6831	3253	109(5)
C(7)	10046	7312	3006	112(5)
C(6)	9943	7098	2287	113(5)
C(5)	9547	6402	1816	111(5)
C(4)	9254	5921	2063	109(5)
C(9)	7305	3296	1242	128(5)
C(10)	8035	3176	1530	137(6)
C(12)	8787	2946	565	148(6)
C(13)	9037	3137	69	150(6)
C(14)	8838	3762	9	151(7)
C(15)	8388	4198	445	150(6)
C(16)	8137	4007	942	148(6)
C(11)	8337	3381	1002	145(6)
C(17)	5552	1198	1708	85(4)
C(18)	5458	556	1908	94(4)
C(19)	5123	-160	1270	101(4)
C(20)	4420	-464	1176	105(5)
C(21)	4155	-1167	606	107(5)
C(22)	4594	-1565	131	108(5)
C(23)	5297	-1260	226	108(5)
C(24)	5562	-558	796	105(5)
C(25)	3113	735	1009	111(5)
C(26)	3432	599	347	120(5)
C(27)	2882	28	-250	127(5)
C(32)	2723	366	-681	130(6)
C(31)	2302	-55	-1334	132(6)
C(30)	2040	-813	-1557	133(6)

C(29)	2200	-1150	-1126	132(6)
C(28)	2621	-730	-473	129(6)
C(33)	3506	446	3371	132(5)
C(34)	3044	59	3724	145(6)
C(35)	3037	-773	3441	154(6)
C(40)	2691	-1369	2809	157(6)
C(39)	2786	-2112	2641	159(7)
C(38)	3227	-2260	3104	159(7)
C(37)	3572	-1664	3736	159(7)
C(36)	3477	-921	3904	157(6)
C(41)	1690	1682	5320	123(5)
C(42)	2210	1295	5555	131(5)
C(48)	2776	1383	6591	140(6)
C(47)	3045	1818	7303	140(6)
C(46)	2678	2372	7742	142(6)
C(45)	2042	2492	7470	141(6)
C(44)	1773	2057	6758	139(6)
C(43)	2140	1503	6318	137(6)
C(49)	3904	4250	8148	167(7)
C(50)	3849	3574	8287	174(7)
C(52)	4665	4342	9556	178(8)
C(53)	5253	4316	9971	179(8)
C(54)	5622	3700	9710	179(8)
C(55)	5403	3109	9033	178(8)
C(56)	4814	3135	8618	178(8)
C(51)	4446	3751	8879	177(7)
C(57)	1717	1605	3285	88(4)
C(58)	1216	1046	2628	98(4)
C(59)	760	460	2757	106(5)
C(60)	197	656	3134	109(5)
C(61)	-198	118	3255	112(5)
C(62)	-31	-615	2998	113(5)
C(63)	531	-811	2621	113(5)
C(64)	927	-273	2501	110(5)
C(65)	1258	3871	4318	70(3)
C(66)	692	4179	4764	75(4)
C(67)	217	3649	4934	79(4)
C(72)	254	2875	4598	83(4)

C(71)	-227	2372	4687	83(5)
C(70)	-744	2644	5111	83(5)
C(69)	-780	3418	5447	82(5)
C(68)	-300	3921	5358	81(4)
C(73)	2389	6651	6632	66(3)
C(74)	1727	6778	6268	72(4)
C(75)	1117	6910	6683	77(4)
C(76)	888	7614	7009	79(4)
C(77)	312	7696	7369	80(4)
C(78)	-36	7073	7404	83(4)
C(79)	193	6370	7078	82(4)
C(80)	769	6288	6717	79(4)
C(81)	2701	7177	4761	84(4)
C(82)	3229	7859	5285	87(4)
C(83)	2846	8417	5846	92(4)
C(88)	2958	8511	6533	93(5)
C(87)	2638	9045	7052	96(5)
C(86)	2206	9485	6884	96(5)
C(85)	2095	9390	6197	96(5)
C(84)	2415	8856	5678	94(5)
C(89)	5392	7937	4253	89(4)
C(90)	4908	8435	4116	98(4)
C(91)	5145	8835	3698	103(5)
C(92)	5459	9549	4220	106(5)
C(93)	5764	10080	4034	109(5)
C(94)	5755	9897	3326	108(5)
C(95)	5440	9183	2804	107(5)
C(96)	5136	8652	2990	106(5)
C(97)	3681	6167	2182	128(5)
C(98)	3478	6835	2051	139(6)
C(99)	3231	7386	1727	147(6)
C(100)	3270	8160	1941	150(6)
C(101)	2745	8432	1664	152(7)
C(102)	2181	7929	1173	153(7)
C(103)	2143	7155	960	152(7)
C(104)	2668	6883	1237	150(6)
C(105)	3888	3451	883	122(5)
C(106)	3723	3870	462	131(5)

C(107)	3074	3403	-71	138(6)
C(108)	2562	3882	88	140(6)
C(109)	1852	3581	-147	141(6)
C(110)	1654	2801	-541	142(6)
C(111)	2166	2321	-700	142(6)
C(112)	2876	2622	-466	140(6)
C(113)	1516	1811	1172	149(6)
C(114)	1142	1696	465	158(6)
C(115)	858	875	49	164(7)
C(120)	978	547	495	167(7)
C(119)	765	-225	249	169(7)
C(118)	434	-670	-442	169(7)
C(117)	314	-342	-888	168(7)
C(116)	527	430	-642	167(7)
C(121)	609	5454	2580	152(6)
C(122)	1154	6095	2608	161(6)
C(123)	1074	5816	1852	167(7)
C(128)	422	5445	1445	170(7)
C(127)	345	5147	714	171(7)
C(126)	921	5220	391	172(7)
C(125)	1573	5590	799	171(7)
C(124)	1650	5888	1529	169(7)

Table 3. Bond lengths [Å] and angles [°] for $Au_{52}(PET)_{32}$.

Au(1)-Au(2)	3.0192
Au(1)-Au(3)	2.7473
Au(1)-Au(4)	2.7359
Au(1)-Au(5)	2.9863
Au(1)-Au(6)	2.8094
Au(1)-Au(7)	2.7853
Au(1)-Au(8)	2.9354
Au(1)-Au(9)	2.9303
Au(1)-Au(14)#1	2.8517
Au(1)-Au(22)	2.7237
Au(1)-Au(23)	3.3267
Au(2)-Au(3)	2.9081
Au(2)-Au(7)	2.9318
Au(2)-Au(8)	2.8914
Au(2)-Au(15)#1	2.7506
Au(2)-Au(16)#1	2.7481
Au(2)-Au(19)	3.0447
Au(2)-Au(23)	3.3128
Au(2)-S(8)	2.4001
Au(3)-Au(4)	2.6919
Au(3)-Au(14)#1	2.8538
Au(3)-Au(15)#1	2.9501
Au(3)-Au(19)	3.2107
Au(3)-Au(23)	3.0843
Au(3)-S(5)	2.3689
Au(4)-Au(5)	2.9630
Au(4)-Au(13)#1	2.9291
Au(4)-Au(14)#1	2.8771
Au(4)-Au(18)	3.2699
Au(4)-Au(24)	3.0401
Au(4)-S(3)	2.3453
Au(5)-Au(6)	2.9051
Au(5)-Au(9)	2.8666
Au(5)-Au(13)#1	2.7761
Au(5)-Au(18)	3.2506
Au(5)-Au(21)#1	2.7298

Au(5)-Au(24)	3.1666
Au(5)-S(14)	2.3808
Au(6)-Au(7)	2.7208
Au(6)-Au(9)	3.0411
Au(6)-Au(10)	3.0987
Au(6)-Au(11)	3.0179
Au(6)-Au(22)	2.7295
Au(6)-S(13)	2.3896
Au(7)-Au(8)	3.0477
Au(7)-Au(11)	3.0570
Au(7)-Au(12)	3.0465
Au(7)-Au(22)	2.7697
Au(7)-Au(25)	3.2927
Au(7)-S(9)	2.3439
Au(8)-Au(9)#1	2.8942
Au(8)-Au(9)	3.0514
Au(8)-Au(11)	2.7384
Au(8)-Au(12)	3.1788
Au(8)-Au(13)	3.0046
Au(8)-Au(14)#1	2.8886
Au(8)-Au(14)	2.8942
Au(8)-Au(15)#1	2.9033
Au(8)-Au(16)#1	2.8024
Au(9)-Au(8)#1	2.8942
Au(9)-Au(10)	3.1801
Au(9)-Au(11)	2.7660
Au(9)-Au(13)#1	2.8839
Au(9)-Au(14)	2.9049
Au(9)-Au(14)#1	2.9008
Au(9)-Au(15)	2.9678
Au(9)-Au(21)#1	2.8161
Au(10)-Au(11)	3.1773
Au(10)-Au(15)	3.3712
Au(10)-Au(21)#1	3.0444
Au(10)-S(12)	2.2860
Au(10)-S(13)	2.3040
Au(11)-Au(12)	3.0381
Au(11)-Au(14)	2.7777

Au(11)-S(11)	2.3670
Au(12)-Au(16)#1	3.1573
Au(12)-S(9)	2.3190
Au(12)-S(10)	2.3035
Au(13)-Au(4)#1	2.9290
Au(13)-Au(5)#1	2.7761
Au(13)-Au(9)#1	2.8838
Au(13)-Au(14)	3.0276
Au(13)-Au(16)#1	2.9590
Au(13)-Au(17)#1	3.1408
Au(13)-Au(18)#1	3.2895
Au(13)-Au(21)	2.7765
Au(13)-S(10)	2.4015
Au(14)-Au(1)#1	2.8517
Au(14)-Au(3)#1	2.8538
Au(14)-Au(4)#1	2.8770
Au(14)-Au(8)#1	2.8886
Au(14)-Au(9)#1	2.9007
Au(14)-Au(15)	3.0270
Au(15)-Au(2)#1	2.7505
Au(15)-Au(3)#1	2.9501
Au(15)-Au(8)#1	2.9033
Au(15)-Au(16)	2.7485
Au(15)-Au(19)#1	3.1516
Au(15)-Au(20)#1	3.2206
Au(15)-Au(21)#1	2.9708
Au(15)-S(12)	2.4001
Au(16)-Au(2)#1	2.7480
Au(16)-Au(8)#1	2.8023
Au(16)-Au(12)#1	3.1572
Au(16)-Au(13)#1	2.9590
Au(16)-Au(17)	3.3534
Au(16)-Au(20)#1	3.1150
Au(16)-Au(21)#1	2.9628
Au(16)-S(1)	2.3415
Au(17)-Au(13)#1	3.1408
Au(17)-Au(18)	3.1759
Au(17)-Au(21)#1	3.1242

Au(17)-S(1)	2.2998
Au(17)-S(2)	2.3375
Au(18)-Au(13)#1	3.2895
Au(18)-S(2)	2.3079
Au(18)-S(3)	2.3178
Au(19)-Au(15)#1	3.1515
Au(19)-Au(20)	3.2901
Au(19)-S(5)	2.2924
Au(19)-S(6)	2.2635
Au(20)-Au(15)#1	3.2207
Au(20)-Au(16)#1	3.1150
Au(20)-Au(21)	3.2355
Au(20)-S(6)	2.3135
Au(20)-S(7)	2.2659
Au(21)-Au(5)#1	2.7298
Au(21)-Au(9)#1	2.8162
Au(21)-Au(10)#1	3.0444
Au(21)-Au(15)#1	2.9709
Au(21)-Au(16)#1	2.9628
Au(21)-Au(17)#1	3.1241
Au(21)-S(7)	2.3446
Au(22)-Au(23)	2.8648
Au(22)-Au(24)	2.9771
Au(22)-Au(26)	2.9427
Au(22)-S(15)	2.3520
Au(23)-S(4)	2.2731
Au(23)-S(8)	2.2634
Au(24)-S(4)	2.3325
Au(24)-S(14)	2.3038
Au(25)-S(11)	2.2844
Au(25)-S(16)	2.2609
Au(26)-S(15)	2.2802
Au(26)-S(16)	2.2984
S(1)-C(1)	1.7756
S(2)-C(9)	1.8148
S(3)-C(17)	1.7916
S(4)-C(25)	1.7734
S(5)-C(33)	1.8225

S(6)-C(41)	1.7917
S(7)-C(49)	1.7857
S(8)-C(57)	1.7611
S(9)-C(65)	1.7952
S(10)-C(73)	1.7893
S(11)-C(81)	1.7843
S(12)-C(89)	1.8008
S(13)-C(97)	1.8706
S(14)-C(105)	1.8003
S(15)-C(113)	1.8000
S(16)-C(121)	1.8025
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(1)-C(2)	1.5118
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-C(3)	1.5214
C(3)-C(8)	1.3900
C(3)-C(4)	1.3900
C(8)-H(8)	0.9500
C(8)-C(7)	1.3900
C(7)-H(7)	0.9500
C(7)-C(6)	1.3900
C(6)-H(6)	0.9500
C(6)-C(5)	1.3900
C(5)-H(5)	0.9500
C(5)-C(4)	1.3900
C(4)-H(4)	0.9500
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(9)-C(10)	1.5589
C(10)-C(11)	1.5103
C(12)-C(13)	1.3900
C(12)-C(11)	1.3900
C(13)-C(14)	1.3900
C(14)-C(15)	1.3900
C(15)-C(16)	1.3900
C(16)-C(11)	1.3900

C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.5205
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(18)-C(19)	1.4961
C(19)-C(20)	1.3900
C(19)-C(24)	1.3900
C(20)-H(20)	0.9500
C(20)-C(21)	1.3900
C(21)-H(21)	0.9500
C(21)-C(22)	1.3900
C(22)-H(22)	0.9500
C(22)-C(23)	1.3900
C(23)-H(23)	0.9500
C(23)-C(24)	1.3900
C(24)-H(24)	0.9500
C(25)-C(26)	1.5207
C(26)-C(27)	1.5084
C(27)-C(32)	1.3900
C(27)-C(28)	1.3900
C(32)-H(32)	0.9500
C(32)-C(31)	1.3900
C(31)-H(31)	0.9500
C(31)-C(30)	1.3900
C(30)-H(30)	0.9500
C(30)-C(29)	1.3900
C(29)-H(29)	0.9500
C(29)-C(28)	1.3900
C(28)-H(28)	0.9500
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(33)-C(34)	1.5749
C(34)-C(35)	1.4845
C(35)-C(40)	1.3900
C(35)-C(36)	1.3900
C(40)-C(39)	1.3900
C(39)-C(38)	1.3900

C(38)-C(37)	1.3900
C(37)-C(36)	1.3900
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(41)-C(42)	1.4930
C(42)-C(43)	1.5198
C(48)-C(47)	1.3900
C(48)-C(43)	1.3900
C(47)-C(46)	1.3900
C(46)-C(45)	1.3900
C(45)-C(44)	1.3900
C(44)-C(43)	1.3900
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(49)-C(50)	1.4999
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(50)-C(51)	1.5170
C(52)-H(52)	0.9500
C(52)-C(53)	1.3900
C(52)-C(51)	1.3900
C(53)-H(53)	0.9500
C(53)-C(54)	1.3900
C(54)-H(54)	0.9500
C(54)-C(55)	1.3900
C(55)-H(55)	0.9500
C(55)-C(56)	1.3900
C(56)-H(56)	0.9500
C(56)-C(51)	1.3900
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(57)-C(58)	1.5164
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(58)-C(59)	1.5364
C(59)-C(60)	1.3900
C(59)-C(64)	1.3900
C(60)-H(60)	0.9500

C(60)-C(61)	1.3900
C(61)-H(61)	0.9500
C(61)-C(62)	1.3900
C(62)-H(62)	0.9500
C(62)-C(63)	1.3900
C(63)-H(63)	0.9500
C(63)-C(64)	1.3900
C(64)-H(64)	0.9500
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(65)-C(66)	1.5044
C(66)-C(67)	1.5207
C(67)-C(72)	1.3900
C(67)-C(68)	1.3900
C(72)-H(72)	0.9500
C(72)-C(71)	1.3900
C(71)-H(71)	0.9500
C(71)-C(70)	1.3900
C(70)-H(70)	0.9500
C(70)-C(69)	1.3900
C(69)-H(69)	0.9500
C(69)-C(68)	1.3900
C(68)-H(68)	0.9500
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(73)-C(74)	1.5288
C(74)-C(75)	1.5097
C(75)-C(76)	1.3900
C(75)-C(80)	1.3900
C(76)-H(76)	0.9500
C(76)-C(77)	1.3900
C(77)-H(77)	0.9500
C(77)-C(78)	1.3900
C(78)-H(78)	0.9500
C(78)-C(79)	1.3900
C(79)-H(79)	0.9500
C(79)-C(80)	1.3900
C(80)-H(80)	0.9500

C(81)-H(81A)	0.9900
C(81)-H(81B)	0.9900
C(81)-C(82)	1.5195
C(82)-H(82A)	0.9900
C(82)-H(82B)	0.9900
C(82)-C(83)	1.5267
C(83)-C(88)	1.3900
C(83)-C(84)	1.3900
C(88)-H(88)	0.9500
C(88)-C(87)	1.3900
C(87)-H(87)	0.9500
C(87)-C(86)	1.3900
C(86)-H(86)	0.9500
C(86)-C(85)	1.3900
C(85)-H(85)	0.9500
C(85)-C(84)	1.3900
C(84)-H(84)	0.9500
C(89)-H(89A)	0.9900
C(89)-H(89B)	0.9900
C(89)-C(90)	1.5165
C(90)-H(90A)	0.9900
C(90)-H(90B)	0.9900
C(90)-C(91)	1.5156
C(91)-C(92)	1.3900
C(91)-C(96)	1.3900
C(92)-H(92)	0.9500
C(92)-C(93)	1.3900
C(93)-H(93)	0.9500
C(93)-C(94)	1.3900
C(94)-H(94)	0.9500
C(94)-C(95)	1.3900
C(95)-H(95)	0.9500
C(95)-C(96)	1.3900
C(96)-H(96)	0.9500
C(97)-C(98)	1.5485
C(98)-C(99)	1.6175
C(99)-C(100)	1.3900
C(99)-C(104)	1.3900

C(100)-C(101)	1.3900
C(101)-C(102)	1.3900
C(102)-C(103)	1.3900
C(103)-C(104)	1.3900
C(105)-H(10A)	0.9900
C(105)-H(10B)	0.9900
C(105)-C(106)	1.5081
C(106)-C(107)	1.5169
C(107)-C(108)	1.3900
C(107)-C(112)	1.3900
C(108)-H(108)	0.9500
C(108)-C(109)	1.3900
C(109)-H(109)	0.9500
C(109)-C(110)	1.3900
C(110)-H(110)	0.9500
C(110)-C(111)	1.3900
C(111)-H(111)	0.9500
C(111)-C(112)	1.3900
C(112)-H(112)	0.9500
C(113)-H(11A)	0.9900
C(113)-H(11B)	0.9900
C(113)-C(114)	1.5217
C(114)-H(11C)	0.9900
C(114)-H(11D)	0.9900
C(114)-C(115)	1.4859
C(115)-C(120)	1.3900
C(115)-C(116)	1.3900
C(120)-C(119)	1.3900
C(119)-C(118)	1.3900
C(118)-C(117)	1.3900
C(117)-C(116)	1.3900
C(121)-H(12A)	0.9900
C(121)-H(12B)	0.9900
C(121)-C(122)	1.5549
C(122)-H(12C)	0.9900
C(122)-H(12D)	0.9900
C(122)-C(123)	1.4456
C(123)-C(128)	1.3900

C(123)-C(124)	1.3900
C(128)-C(127)	1.3900
C(127)-C(126)	1.3900
C(126)-C(125)	1.3900
C(125)-C(124)	1.3900

Au(2)-Au(1)-Au(23)	62.7
Au(3)-Au(1)-Au(2)	60.4
Au(3)-Au(1)-Au(5)	121.0
Au(3)-Au(1)-Au(6)	174.6
Au(3)-Au(1)-Au(7)	120.4
Au(3)-Au(1)-Au(8)	90.4
Au(3)-Au(1)-Au(9)	121.4
Au(3)-Au(1)-Au(14)#1	61.3
Au(3)-Au(1)-Au(23)	60.1
Au(4)-Au(1)-Au(2)	119.2
Au(4)-Au(1)-Au(3)	58.8
Au(4)-Au(1)-Au(5)	62.2
Au(4)-Au(1)-Au(6)	121.9
Au(4)-Au(1)-Au(7)	173.3
Au(4)-Au(1)-Au(8)	121.7
Au(4)-Au(1)-Au(9)	91.0
Au(4)-Au(1)-Au(14)#1	61.9
Au(4)-Au(1)-Au(23)	87.3
Au(5)-Au(1)-Au(2)	178.4
Au(5)-Au(1)-Au(23)	118.6
Au(6)-Au(1)-Au(2)	118.7
Au(6)-Au(1)-Au(5)	60.1
Au(6)-Au(1)-Au(8)	93.3
Au(6)-Au(1)-Au(9)	63.9
Au(6)-Au(1)-Au(14)#1	124.1
Au(6)-Au(1)-Au(23)	114.5
Au(7)-Au(1)-Au(2)	60.5
Au(7)-Au(1)-Au(5)	118.3
Au(7)-Au(1)-Au(6)	58.2
Au(7)-Au(1)-Au(8)	64.3
Au(7)-Au(1)-Au(9)	94.7
Au(7)-Au(1)-Au(14)#1	124.2

Au(7)-Au(1)-Au(23)	86.8
Au(8)-Au(1)-Au(2)	58.1
Au(8)-Au(1)-Au(5)	120.6
Au(8)-Au(1)-Au(23)	120.8
Au(9)-Au(1)-Au(2)	120.8
Au(9)-Au(1)-Au(5)	58.0
Au(9)-Au(1)-Au(8)	62.7
Au(9)-Au(1)-Au(23)	176.5
Au(14)#1-Au(1)-Au(2)	89.1
Au(14)#1-Au(1)-Au(5)	90.9
Au(14)#1-Au(1)-Au(8)	59.9
Au(14)#1-Au(1)-Au(9)	60.2
Au(14)#1-Au(1)-Au(23)	121.4
Au(22)-Au(1)-Au(2)	92.2
Au(22)-Au(1)-Au(3)	115.5
Au(22)-Au(1)-Au(4)	113.4
Au(22)-Au(1)-Au(5)	88.0
Au(22)-Au(1)-Au(6)	59.1
Au(22)-Au(1)-Au(7)	60.4
Au(22)-Au(1)-Au(8)	124.6
Au(22)-Au(1)-Au(9)	122.7
Au(22)-Au(1)-Au(14)#1	175.1
Au(22)-Au(1)-Au(23)	55.4
Au(1)-Au(2)-Au(19)	120.1
Au(1)-Au(2)-Au(23)	63.2
Au(3)-Au(2)-Au(1)	55.2
Au(3)-Au(2)-Au(7)	110.6
Au(3)-Au(2)-Au(19)	65.2
Au(3)-Au(2)-Au(23)	59.0
Au(7)-Au(2)-Au(1)	55.8
Au(7)-Au(2)-Au(19)	166.8
Au(7)-Au(2)-Au(23)	84.8
Au(8)-Au(2)-Au(1)	59.5
Au(8)-Au(2)-Au(3)	88.2
Au(8)-Au(2)-Au(7)	63.1
Au(8)-Au(2)-Au(19)	127.5
Au(8)-Au(2)-Au(23)	122.7
Au(15)#1-Au(2)-Au(1)	91.0

Au(15)#1-Au(2)-Au(3)	62.8
Au(15)#1-Au(2)-Au(7)	124.7
Au(15)#1-Au(2)-Au(8)	61.9
Au(15)#1-Au(2)-Au(19)	65.7
Au(15)#1-Au(2)-Au(23)	121.1
Au(16)#1-Au(2)-Au(1)	119.0
Au(16)#1-Au(2)-Au(3)	122.3
Au(16)#1-Au(2)-Au(7)	96.2
Au(16)#1-Au(2)-Au(8)	59.5
Au(16)#1-Au(2)-Au(15)#1	60.0
Au(16)#1-Au(2)-Au(19)	96.4
Au(16)#1-Au(2)-Au(23)	177.7
Au(19)-Au(2)-Au(23)	82.5
S(8)-Au(2)-Au(1)	95.4
S(8)-Au(2)-Au(3)	100.5
S(8)-Au(2)-Au(7)	79.3
S(8)-Au(2)-Au(8)	141.9
S(8)-Au(2)-Au(15)#1	153.6
S(8)-Au(2)-Au(16)#1	135.0
S(8)-Au(2)-Au(19)	89.1
S(8)-Au(2)-Au(23)	43.1
Au(1)-Au(3)-Au(2)	64.5
Au(1)-Au(3)-Au(14)#1	61.2
Au(1)-Au(3)-Au(15)#1	92.6
Au(1)-Au(3)-Au(19)	123.5
Au(1)-Au(3)-Au(23)	69.3
Au(2)-Au(3)-Au(15)#1	56.0
Au(2)-Au(3)-Au(19)	59.4
Au(2)-Au(3)-Au(23)	67.0
Au(4)-Au(3)-Au(1)	60.4
Au(4)-Au(3)-Au(2)	124.8
Au(4)-Au(3)-Au(14)#1	62.4
Au(4)-Au(3)-Au(15)#1	125.3
Au(4)-Au(3)-Au(19)	173.1
Au(4)-Au(3)-Au(23)	93.2
Au(14)#1-Au(3)-Au(2)	91.3
Au(14)#1-Au(3)-Au(15)#1	62.8
Au(14)#1-Au(3)-Au(19)	124.1

Au(14)#1-Au(3)-Au(23)	130.5
Au(15)#1-Au(3)-Au(19)	61.4
Au(15)#1-Au(3)-Au(23)	122.3
Au(23)-Au(3)-Au(19)	83.6
S(5)-Au(3)-Au(1)	160.6
S(5)-Au(3)-Au(2)	103.9
S(5)-Au(3)-Au(4)	128.8
S(5)-Au(3)-Au(14)#1	137.1
S(5)-Au(3)-Au(15)#1	92.9
S(5)-Au(3)-Au(19)	45.5
S(5)-Au(3)-Au(23)	92.2
Au(1)-Au(4)-Au(5)	63.1
Au(1)-Au(4)-Au(13)#1	91.8
Au(1)-Au(4)-Au(14)#1	61.0
Au(1)-Au(4)-Au(18)	125.2
Au(1)-Au(4)-Au(24)	73.1
Au(3)-Au(4)-Au(1)	60.8
Au(3)-Au(4)-Au(5)	123.9
Au(3)-Au(4)-Au(13)#1	124.4
Au(3)-Au(4)-Au(14)#1	61.5
Au(3)-Au(4)-Au(18)	171.1
Au(3)-Au(4)-Au(24)	100.1
Au(5)-Au(4)-Au(18)	62.6
Au(5)-Au(4)-Au(24)	63.7
Au(13)#1-Au(4)-Au(5)	56.2
Au(13)#1-Au(4)-Au(18)	63.8
Au(13)#1-Au(4)-Au(24)	118.0
Au(14)#1-Au(4)-Au(5)	90.9
Au(14)#1-Au(4)-Au(13)#1	62.9
Au(14)#1-Au(4)-Au(18)	126.5
Au(14)#1-Au(4)-Au(24)	134.0
Au(24)-Au(4)-Au(18)	77.0
S(3)-Au(4)-Au(1)	163.9
S(3)-Au(4)-Au(3)	127.2
S(3)-Au(4)-Au(5)	107.4
S(3)-Au(4)-Au(13)#1	92.8
S(3)-Au(4)-Au(14)#1	134.3
S(3)-Au(4)-Au(18)	45.1

S(3)-Au(4)-Au(24)	91.1
Au(1)-Au(5)-Au(18)	117.6
Au(1)-Au(5)-Au(24)	68.1
Au(4)-Au(5)-Au(1)	54.8
Au(4)-Au(5)-Au(18)	63.3
Au(4)-Au(5)-Au(24)	59.4
Au(6)-Au(5)-Au(1)	56.9
Au(6)-Au(5)-Au(4)	111.4
Au(6)-Au(5)-Au(18)	165.9
Au(6)-Au(5)-Au(24)	90.6
Au(9)-Au(5)-Au(1)	60.0
Au(9)-Au(5)-Au(4)	87.8
Au(9)-Au(5)-Au(6)	63.6
Au(9)-Au(5)-Au(18)	126.9
Au(9)-Au(5)-Au(24)	128.1
Au(13)#1-Au(5)-Au(1)	89.8
Au(13)#1-Au(5)-Au(4)	61.3
Au(13)#1-Au(5)-Au(6)	124.7
Au(13)#1-Au(5)-Au(9)	61.4
Au(13)#1-Au(5)-Au(18)	65.6
Au(13)#1-Au(5)-Au(24)	118.7
Au(21)#1-Au(5)-Au(1)	120.4
Au(21)#1-Au(5)-Au(4)	121.6
Au(21)#1-Au(5)-Au(6)	97.0
Au(21)#1-Au(5)-Au(9)	60.4
Au(21)#1-Au(5)-Au(13)#1	60.6
Au(21)#1-Au(5)-Au(18)	96.7
Au(21)#1-Au(5)-Au(24)	170.9
Au(24)-Au(5)-Au(18)	75.5
S(14)-Au(5)-Au(1)	110.2
S(14)-Au(5)-Au(4)	99.4
S(14)-Au(5)-Au(6)	97.4
S(14)-Au(5)-Au(9)	161.0
S(14)-Au(5)-Au(13)#1	137.3
S(14)-Au(5)-Au(18)	71.7
S(14)-Au(5)-Au(21)#1	127.0
S(14)-Au(5)-Au(24)	46.5
Au(1)-Au(6)-Au(5)	63.0

Au(1)-Au(6)-Au(9)	60.0
Au(1)-Au(6)-Au(10)	122.3
Au(1)-Au(6)-Au(11)	85.1
Au(5)-Au(6)-Au(9)	57.6
Au(5)-Au(6)-Au(10)	85.4
Au(5)-Au(6)-Au(11)	111.9
Au(7)-Au(6)-Au(1)	60.5
Au(7)-Au(6)-Au(5)	123.4
Au(7)-Au(6)-Au(9)	93.5
Au(7)-Au(6)-Au(10)	125.9
Au(7)-Au(6)-Au(11)	64.1
Au(7)-Au(6)-Au(22)	61.1
Au(9)-Au(6)-Au(10)	62.4
Au(11)-Au(6)-Au(9)	54.3
Au(11)-Au(6)-Au(10)	62.6
Au(22)-Au(6)-Au(1)	58.9
Au(22)-Au(6)-Au(5)	89.5
Au(22)-Au(6)-Au(9)	118.6
Au(22)-Au(6)-Au(10)	173.0
Au(22)-Au(6)-Au(11)	124.0
S(13)-Au(6)-Au(1)	147.9
S(13)-Au(6)-Au(5)	85.0
S(13)-Au(6)-Au(7)	151.5
S(13)-Au(6)-Au(9)	102.1
S(13)-Au(6)-Au(10)	47.5
S(13)-Au(6)-Au(11)	106.4
S(13)-Au(6)-Au(22)	127.3
Au(1)-Au(7)-Au(2)	63.7
Au(1)-Au(7)-Au(8)	60.2
Au(1)-Au(7)-Au(11)	84.7
Au(1)-Au(7)-Au(12)	123.1
Au(1)-Au(7)-Au(25)	130.6
Au(2)-Au(7)-Au(8)	57.8
Au(2)-Au(7)-Au(11)	111.0
Au(2)-Au(7)-Au(12)	87.9
Au(2)-Au(7)-Au(25)	164.2
Au(6)-Au(7)-Au(1)	61.3
Au(6)-Au(7)-Au(2)	125.0

Au(6)-Au(7)-Au(8)	92.7
Au(6)-Au(7)-Au(11)	62.7
Au(6)-Au(7)-Au(12)	120.9
Au(6)-Au(7)-Au(22)	59.6
Au(6)-Au(7)-Au(25)	69.5
Au(8)-Au(7)-Au(11)	53.3
Au(8)-Au(7)-Au(25)	120.1
Au(11)-Au(7)-Au(25)	68.3
Au(12)-Au(7)-Au(8)	62.9
Au(12)-Au(7)-Au(11)	59.7
Au(12)-Au(7)-Au(25)	78.2
Au(22)-Au(7)-Au(1)	58.7
Au(22)-Au(7)-Au(2)	93.1
Au(22)-Au(7)-Au(8)	118.9
Au(22)-Au(7)-Au(11)	121.2
Au(22)-Au(7)-Au(12)	178.2
Au(22)-Au(7)-Au(25)	100.5
S(9)-Au(7)-Au(1)	158.5
S(9)-Au(7)-Au(2)	94.9
S(9)-Au(7)-Au(6)	139.8
S(9)-Au(7)-Au(8)	107.3
S(9)-Au(7)-Au(11)	101.8
S(9)-Au(7)-Au(12)	48.9
S(9)-Au(7)-Au(22)	129.5
S(9)-Au(7)-Au(25)	70.3
Au(1)-Au(8)-Au(7)	55.4
Au(1)-Au(8)-Au(9)	58.6
Au(1)-Au(8)-Au(12)	114.0
Au(1)-Au(8)-Au(13)	177.4
Au(2)-Au(8)-Au(1)	62.4
Au(2)-Au(8)-Au(7)	59.1
Au(2)-Au(8)-Au(9)	121.0
Au(2)-Au(8)-Au(9)#1	118.3
Au(2)-Au(8)-Au(12)	86.1
Au(2)-Au(8)-Au(13)	118.8
Au(2)-Au(8)-Au(14)	178.0
Au(2)-Au(8)-Au(15)#1	56.7
Au(7)-Au(8)-Au(9)	87.1

Au(7)-Au(8)-Au(12)	58.5
Au(9)#1-Au(8)-Au(1)	118.9
Au(9)#1-Au(8)-Au(7)	174.3
Au(9)#1-Au(8)-Au(9)	90.4
Au(9)-Au(8)-Au(12)	117.6
Au(9)#1-Au(8)-Au(12)	127.1
Au(9)#1-Au(8)-Au(13)	58.5
Au(9)#1-Au(8)-Au(15)#1	61.6
Au(11)-Au(8)-Au(1)	88.0
Au(11)-Au(8)-Au(2)	122.5
Au(11)-Au(8)-Au(7)	63.5
Au(11)-Au(8)-Au(9)#1	119.2
Au(11)-Au(8)-Au(9)	56.8
Au(11)-Au(8)-Au(12)	61.3
Au(11)-Au(8)-Au(13)	93.1
Au(11)-Au(8)-Au(14)#1	115.1
Au(11)-Au(8)-Au(14)	59.0
Au(11)-Au(8)-Au(15)#1	177.6
Au(11)-Au(8)-Au(16)#1	124.3
Au(13)-Au(8)-Au(7)	127.1
Au(13)-Au(8)-Au(9)	120.1
Au(13)-Au(8)-Au(12)	68.6
Au(14)#1-Au(8)-Au(1)	58.6
Au(14)-Au(8)-Au(1)	117.0
Au(14)#1-Au(8)-Au(2)	91.0
Au(14)#1-Au(8)-Au(7)	114.1
Au(14)-Au(8)-Au(7)	122.4
Au(14)#1-Au(8)-Au(9)	58.4
Au(14)#1-Au(8)-Au(9)#1	60.3
Au(14)-Au(8)-Au(9)	58.4
Au(14)-Au(8)-Au(9)#1	60.1
Au(14)-Au(8)-Au(12)	95.8
Au(14)#1-Au(8)-Au(12)	172.5
Au(14)#1-Au(8)-Au(13)	118.8
Au(14)-Au(8)-Au(13)	61.7
Au(14)#1-Au(8)-Au(14)	87.1
Au(14)-Au(8)-Au(15)#1	121.7
Au(14)#1-Au(8)-Au(15)#1	63.0

Au(15)#1-Au(8)-Au(1)	89.8
Au(15)#1-Au(8)-Au(7)	115.5
Au(15)#1-Au(8)-Au(9)	121.4
Au(15)#1-Au(8)-Au(12)	120.4
Au(15)#1-Au(8)-Au(13)	89.2
Au(16)#1-Au(8)-Au(1)	120.1
Au(16)#1-Au(8)-Au(2)	57.7
Au(16)#1-Au(8)-Au(7)	92.5
Au(16)#1-Au(8)-Au(9)#1	89.8
Au(16)#1-Au(8)-Au(9)	178.5
Au(16)#1-Au(8)-Au(12)	63.4
Au(16)#1-Au(8)-Au(13)	61.2
Au(16)#1-Au(8)-Au(14)	122.9
Au(16)#1-Au(8)-Au(14)#1	120.6
Au(16)#1-Au(8)-Au(15)#1	57.6
Au(1)-Au(9)-Au(6)	56.1
Au(1)-Au(9)-Au(8)	58.7
Au(1)-Au(9)-Au(10)	115.8
Au(1)-Au(9)-Au(15)	177.8
Au(5)-Au(9)-Au(1)	62.0
Au(5)-Au(9)-Au(6)	58.8
Au(5)-Au(9)-Au(8)#1	120.4
Au(5)-Au(9)-Au(8)	120.7
Au(5)-Au(9)-Au(10)	84.6
Au(5)-Au(9)-Au(13)#1	57.7
Au(5)-Au(9)-Au(14)#1	92.4
Au(5)-Au(9)-Au(14)	178.8
Au(5)-Au(9)-Au(15)	119.2
Au(6)-Au(9)-Au(8)	86.6
Au(6)-Au(9)-Au(10)	59.7
Au(8)#1-Au(9)-Au(1)	118.5
Au(8)#1-Au(9)-Au(6)	174.5
Au(8)#1-Au(9)-Au(8)	89.6
Au(8)-Au(9)-Au(10)	119.7
Au(8)#1-Au(9)-Au(10)	125.8
Au(8)#1-Au(9)-Au(14)#1	59.9
Au(8)#1-Au(9)-Au(14)	59.8
Au(8)#1-Au(9)-Au(15)	59.4

Au(11)-Au(9)-Au(1)	87.5
Au(11)-Au(9)-Au(5)	121.2
Au(11)-Au(9)-Au(6)	62.4
Au(11)-Au(9)-Au(8)	55.9
Au(11)-Au(9)-Au(8)#1	118.3
Au(11)-Au(9)-Au(10)	64.2
Au(11)-Au(9)-Au(13)#1	176.3
Au(11)-Au(9)-Au(14)	58.6
Au(11)-Au(9)-Au(14)#1	113.9
Au(11)-Au(9)-Au(15)	93.2
Au(11)-Au(9)-Au(21)#1	124.7
Au(13)#1-Au(9)-Au(1)	88.9
Au(13)#1-Au(9)-Au(6)	116.2
Au(13)#1-Au(9)-Au(8)	121.0
Au(13)#1-Au(9)-Au(8)#1	62.7
Au(13)#1-Au(9)-Au(10)	118.6
Au(13)#1-Au(9)-Au(14)#1	63.1
Au(13)#1-Au(9)-Au(14)	122.4
Au(13)#1-Au(9)-Au(15)	90.3
Au(14)-Au(9)-Au(1)	116.8
Au(14)#1-Au(9)-Au(1)	58.6
Au(14)-Au(9)-Au(6)	120.9
Au(14)#1-Au(9)-Au(6)	114.6
Au(14)#1-Au(9)-Au(8)	58.0
Au(14)-Au(9)-Au(8)	58.1
Au(14)#1-Au(9)-Au(10)	174.3
Au(14)-Au(9)-Au(10)	96.3
Au(14)#1-Au(9)-Au(14)	86.7
Au(14)-Au(9)-Au(15)	62.0
Au(14)#1-Au(9)-Au(15)	119.3
Au(15)-Au(9)-Au(6)	126.1
Au(15)-Au(9)-Au(8)	120.1
Au(15)-Au(9)-Au(10)	66.4
Au(21)#1-Au(9)-Au(1)	119.4
Au(21)#1-Au(9)-Au(5)	57.4
Au(21)#1-Au(9)-Au(6)	92.2
Au(21)#1-Au(9)-Au(8)	178.1
Au(21)#1-Au(9)-Au(8)#1	91.5

Au(21)#1-Au(9)-Au(10)	60.7
Au(21)#1-Au(9)-Au(13)#1	58.3
Au(21)#1-Au(9)-Au(14)#1	121.4
Au(21)#1-Au(9)-Au(14)	123.8
Au(21)#1-Au(9)-Au(15)	61.7
Au(6)-Au(10)-Au(9)	57.9
Au(6)-Au(10)-Au(11)	57.5
Au(6)-Au(10)-Au(15)	111.7
Au(9)-Au(10)-Au(15)	53.8
Au(11)-Au(10)-Au(9)	51.6
Au(11)-Au(10)-Au(15)	79.0
Au(21)#1-Au(10)-Au(6)	86.9
Au(21)#1-Au(10)-Au(9)	53.7
Au(21)#1-Au(10)-Au(11)	105.2
Au(21)#1-Au(10)-Au(15)	54.9
S(12)-Au(10)-Au(6)	138.6
S(12)-Au(10)-Au(9)	91.3
S(12)-Au(10)-Au(11)	82.1
S(12)-Au(10)-Au(15)	45.4
S(12)-Au(10)-Au(21)#1	96.5
S(12)-Au(10)-S(13)	168.5
S(13)-Au(10)-Au(6)	49.9
S(13)-Au(10)-Au(9)	100.1
S(13)-Au(10)-Au(11)	103.8
S(13)-Au(10)-Au(15)	144.9
S(13)-Au(10)-Au(21)#1	91.6
Au(6)-Au(11)-Au(7)	53.2
Au(6)-Au(11)-Au(10)	60.0
Au(6)-Au(11)-Au(12)	111.9
Au(7)-Au(11)-Au(10)	112.5
Au(8)-Au(11)-Au(6)	93.0
Au(8)-Au(11)-Au(7)	63.2
Au(8)-Au(11)-Au(9)	67.3
Au(8)-Au(11)-Au(10)	131.2
Au(8)-Au(11)-Au(12)	66.5
Au(8)-Au(11)-Au(14)	63.3
Au(9)-Au(11)-Au(6)	63.3
Au(9)-Au(11)-Au(7)	92.3

Au(9)-Au(11)-Au(10)	64.3
Au(9)-Au(11)-Au(12)	133.2
Au(9)-Au(11)-Au(14)	63.2
Au(12)-Au(11)-Au(7)	60.0
Au(12)-Au(11)-Au(10)	157.9
Au(14)-Au(11)-Au(6)	126.4
Au(14)-Au(11)-Au(7)	126.3
Au(14)-Au(11)-Au(10)	99.0
Au(14)-Au(11)-Au(12)	101.6
S(11)-Au(11)-Au(6)	86.6
S(11)-Au(11)-Au(7)	97.9
S(11)-Au(11)-Au(8)	155.5
S(11)-Au(11)-Au(9)	132.4
S(11)-Au(11)-Au(10)	68.9
S(11)-Au(11)-Au(12)	90.9
S(11)-Au(11)-Au(14)	134.6
Au(7)-Au(12)-Au(8)	58.6
Au(7)-Au(12)-Au(16)#1	85.9
Au(11)-Au(12)-Au(7)	60.3
Au(11)-Au(12)-Au(8)	52.2
Au(11)-Au(12)-Au(16)#1	104.5
Au(16)#1-Au(12)-Au(8)	52.5
S(9)-Au(12)-Au(7)	49.6
S(9)-Au(12)-Au(8)	103.9
S(9)-Au(12)-Au(11)	103.0
S(9)-Au(12)-Au(16)#1	98.7
S(10)-Au(12)-Au(7)	140.9
S(10)-Au(12)-Au(8)	89.7
S(10)-Au(12)-Au(11)	82.7
S(10)-Au(12)-Au(16)#1	92.0
S(10)-Au(12)-S(9)	166.0
Au(4)#1-Au(13)-Au(8)	115.1
Au(4)#1-Au(13)-Au(14)	57.7
Au(4)#1-Au(13)-Au(16)#1	171.1
Au(4)#1-Au(13)-Au(17)#1	122.2
Au(4)#1-Au(13)-Au(18)#1	63.1
Au(5)#1-Au(13)-Au(4)#1	62.5
Au(5)#1-Au(13)-Au(8)	119.7

Au(5)#1-Au(13)-Au(9)#1	60.8
Au(5)#1-Au(13)-Au(14)	91.5
Au(5)#1-Au(13)-Au(16)#1	120.9
Au(5)#1-Au(13)-Au(17)#1	90.0
Au(5)#1-Au(13)-Au(18)#1	64.2
Au(5)#1-Au(13)-Au(21)	58.9
Au(8)-Au(13)-Au(14)	57.3
Au(8)-Au(13)-Au(17)#1	122.6
Au(8)-Au(13)-Au(18)#1	175.0
Au(9)#1-Au(13)-Au(4)#1	88.2
Au(9)#1-Au(13)-Au(8)	58.8
Au(9)#1-Au(13)-Au(14)	58.7
Au(9)#1-Au(13)-Au(16)#1	87.0
Au(9)#1-Au(13)-Au(17)#1	123.0
Au(9)#1-Au(13)-Au(18)#1	124.9
Au(14)-Au(13)-Au(17)#1	178.2
Au(14)-Au(13)-Au(18)#1	120.7
Au(16)#1-Au(13)-Au(8)	56.1
Au(16)#1-Au(13)-Au(14)	113.4
Au(16)#1-Au(13)-Au(17)#1	66.6
Au(16)#1-Au(13)-Au(18)#1	125.7
Au(17)#1-Au(13)-Au(18)#1	59.1
Au(21)-Au(13)-Au(4)#1	121.2
Au(21)-Au(13)-Au(8)	90.0
Au(21)-Au(13)-Au(9)#1	59.6
Au(21)-Au(13)-Au(14)	118.3
Au(21)-Au(13)-Au(16)#1	62.1
Au(21)-Au(13)-Au(17)#1	63.4
Au(21)-Au(13)-Au(18)#1	94.8
S(10)-Au(13)-Au(4)#1	84.4
S(10)-Au(13)-Au(5)#1	140.8
S(10)-Au(13)-Au(8)	92.1
S(10)-Au(13)-Au(9)#1	143.1
S(10)-Au(13)-Au(14)	87.2
S(10)-Au(13)-Au(16)#1	95.1
S(10)-Au(13)-Au(17)#1	90.9
S(10)-Au(13)-Au(18)#1	83.1
S(10)-Au(13)-Au(21)	150.3

Au(1)#1-Au(14)-Au(3)#1	57.6
Au(1)#1-Au(14)-Au(4)#1	57.1
Au(1)#1-Au(14)-Au(8)#1	61.5
Au(1)#1-Au(14)-Au(8)	121.2
Au(1)#1-Au(14)-Au(9)#1	61.2
Au(1)#1-Au(14)-Au(9)	121.4
Au(1)#1-Au(14)-Au(13)	87.6
Au(1)#1-Au(14)-Au(15)	88.9
Au(3)#1-Au(14)-Au(4)#1	56.0
Au(3)#1-Au(14)-Au(8)#1	89.3
Au(3)#1-Au(14)-Au(8)	176.4
Au(3)#1-Au(14)-Au(9)#1	118.7
Au(3)#1-Au(14)-Au(9)	120.1
Au(3)#1-Au(14)-Au(13)	115.4
Au(3)#1-Au(14)-Au(15)	60.1
Au(4)#1-Au(14)-Au(8)#1	118.5
Au(4)#1-Au(14)-Au(8)	120.3
Au(4)#1-Au(14)-Au(9)	176.2
Au(4)#1-Au(14)-Au(9)#1	88.8
Au(4)#1-Au(14)-Au(13)	59.4
Au(4)#1-Au(14)-Au(15)	116.2
Au(8)#1-Au(14)-Au(8)	92.9
Au(8)#1-Au(14)-Au(9)#1	63.6
Au(8)-Au(14)-Au(9)#1	59.9
Au(8)-Au(14)-Au(9)	63.5
Au(8)#1-Au(14)-Au(9)	59.9
Au(8)-Au(14)-Au(13)	60.9
Au(8)#1-Au(14)-Au(13)	121.7
Au(8)-Au(14)-Au(15)	123.5
Au(8)#1-Au(14)-Au(15)	58.7
Au(9)#1-Au(14)-Au(9)	93.3
Au(9)-Au(14)-Au(13)	124.4
Au(9)#1-Au(14)-Au(13)	58.2
Au(9)#1-Au(14)-Au(15)	122.3
Au(9)-Au(14)-Au(15)	60.0
Au(11)-Au(14)-Au(1)#1	178.8
Au(11)-Au(14)-Au(3)#1	123.6
Au(11)-Au(14)-Au(4)#1	123.4

Au(11)-Au(14)-Au(8)	57.7
Au(11)-Au(14)-Au(8)#1	118.1
Au(11)-Au(14)-Au(9)	58.2
Au(11)-Au(14)-Au(9)#1	117.6
Au(11)-Au(14)-Au(13)	91.8
Au(11)-Au(14)-Au(15)	91.7
Au(15)-Au(14)-Au(13)	175.5
Au(2)#1-Au(15)-Au(3)#1	61.2
Au(2)#1-Au(15)-Au(8)#1	61.4
Au(2)#1-Au(15)-Au(9)	120.5
Au(2)#1-Au(15)-Au(10)	178.9
Au(2)#1-Au(15)-Au(14)	90.9
Au(2)#1-Au(15)-Au(19)#1	61.7
Au(2)#1-Au(15)-Au(20)#1	91.3
Au(2)#1-Au(15)-Au(21)#1	122.2
Au(3)#1-Au(15)-Au(9)	115.0
Au(3)#1-Au(15)-Au(10)	119.7
Au(3)#1-Au(15)-Au(14)	57.0
Au(3)#1-Au(15)-Au(19)#1	63.4
Au(3)#1-Au(15)-Au(20)#1	125.5
Au(3)#1-Au(15)-Au(21)#1	171.6
Au(8)#1-Au(15)-Au(3)#1	87.2
Au(8)#1-Au(15)-Au(9)	59.1
Au(8)#1-Au(15)-Au(10)	118.9
Au(8)#1-Au(15)-Au(14)	58.3
Au(8)#1-Au(15)-Au(19)#1	123.0
Au(8)#1-Au(15)-Au(20)#1	121.7
Au(8)#1-Au(15)-Au(21)#1	88.3
Au(9)-Au(15)-Au(10)	59.8
Au(9)-Au(15)-Au(14)	58.0
Au(9)-Au(15)-Au(19)#1	176.7
Au(9)-Au(15)-Au(20)#1	119.5
Au(9)-Au(15)-Au(21)#1	56.6
Au(14)-Au(15)-Au(10)	90.1
Au(14)-Au(15)-Au(19)#1	120.4
Au(14)-Au(15)-Au(20)#1	177.3
Au(16)-Au(15)-Au(2)#1	60.0
Au(16)-Au(15)-Au(3)#1	120.8

Au(16)-Au(15)-Au(8)#1	59.4
Au(16)-Au(15)-Au(9)	89.3
Au(16)-Au(15)-Au(10)	119.2
Au(16)-Au(15)-Au(14)	117.6
Au(16)-Au(15)-Au(19)#1	94.0
Au(16)-Au(15)-Au(20)#1	62.3
Au(16)-Au(15)-Au(21)#1	62.3
Au(19)#1-Au(15)-Au(10)	118.1
Au(19)#1-Au(15)-Au(20)#1	62.2
Au(20)#1-Au(15)-Au(10)	87.7
Au(21)#1-Au(15)-Au(10)	57.0
Au(21)#1-Au(15)-Au(14)	114.6
Au(21)#1-Au(15)-Au(19)#1	125.0
Au(21)#1-Au(15)-Au(20)#1	62.9
S(12)-Au(15)-Au(2)#1	137.8
S(12)-Au(15)-Au(3)#1	83.7
S(12)-Au(15)-Au(8)#1	144.6
S(12)-Au(15)-Au(9)	94.4
S(12)-Au(15)-Au(10)	42.7
S(12)-Au(15)-Au(14)	88.6
S(12)-Au(15)-Au(16)	150.6
S(12)-Au(15)-Au(19)#1	82.6
S(12)-Au(15)-Au(20)#1	90.9
S(12)-Au(15)-Au(21)#1	95.9
Au(2)#1-Au(16)-Au(8)#1	62.8
Au(2)#1-Au(16)-Au(12)#1	89.0
Au(2)#1-Au(16)-Au(13)#1	125.5
Au(2)#1-Au(16)-Au(15)	60.1
Au(2)#1-Au(16)-Au(17)	175.2
Au(2)#1-Au(16)-Au(20)#1	93.6
Au(2)#1-Au(16)-Au(21)#1	122.6
Au(8)#1-Au(16)-Au(12)#1	64.1
Au(8)#1-Au(16)-Au(13)#1	62.8
Au(8)#1-Au(16)-Au(17)	122.1
Au(8)#1-Au(16)-Au(20)#1	129.3
Au(8)#1-Au(16)-Au(21)#1	90.4
Au(12)#1-Au(16)-Au(17)	93.4
Au(13)#1-Au(16)-Au(12)#1	69.4

Au(13)#1-Au(16)-Au(17)	59.3
Au(13)#1-Au(16)-Au(20)#1	119.3
Au(13)#1-Au(16)-Au(21)#1	55.9
Au(15)-Au(16)-Au(8)#1	63.1
Au(15)-Au(16)-Au(12)#1	126.6
Au(15)-Au(16)-Au(13)#1	93.2
Au(15)-Au(16)-Au(17)	121.1
Au(15)-Au(16)-Au(20)#1	66.3
Au(15)-Au(16)-Au(21)#1	62.6
Au(20)#1-Au(16)-Au(12)#1	165.6
Au(20)#1-Au(16)-Au(17)	82.9
Au(21)#1-Au(16)-Au(12)#1	125.3
Au(21)#1-Au(16)-Au(17)	58.9
Au(21)#1-Au(16)-Au(20)#1	64.3
S(1)-Au(16)-Au(2)#1	133.5
S(1)-Au(16)-Au(8)#1	140.8
S(1)-Au(16)-Au(12)#1	79.4
S(1)-Au(16)-Au(13)#1	92.2
S(1)-Au(16)-Au(15)	153.6
S(1)-Au(16)-Au(17)	43.2
S(1)-Au(16)-Au(20)#1	88.6
S(1)-Au(16)-Au(21)#1	100.0
Au(13)#1-Au(17)-Au(16)	54.1
Au(13)#1-Au(17)-Au(18)	62.8
Au(18)-Au(17)-Au(16)	116.8
Au(21)#1-Au(17)-Au(13)#1	52.6
Au(21)#1-Au(17)-Au(16)	54.3
Au(21)#1-Au(17)-Au(18)	90.7
S(1)-Au(17)-Au(13)#1	88.4
S(1)-Au(17)-Au(16)	44.2
S(1)-Au(17)-Au(18)	136.7
S(1)-Au(17)-Au(21)#1	96.5
S(1)-Au(17)-S(2)	167.5
S(2)-Au(17)-Au(13)#1	101.7
S(2)-Au(17)-Au(16)	148.2
S(2)-Au(17)-Au(18)	46.5
S(2)-Au(17)-Au(21)#1	95.5
Au(4)-Au(18)-Au(13)#1	53.0

Au(5)-Au(18)-Au(4)	54.1
Au(5)-Au(18)-Au(13)#1	50.2
Au(17)-Au(18)-Au(4)	111.1
Au(17)-Au(18)-Au(5)	81.4
Au(17)-Au(18)-Au(13)#1	58.1
S(2)-Au(18)-Au(4)	141.2
S(2)-Au(18)-Au(5)	88.0
S(2)-Au(18)-Au(13)#1	98.1
S(2)-Au(18)-Au(17)	47.3
S(2)-Au(18)-S(3)	171.8
S(3)-Au(18)-Au(4)	45.8
S(3)-Au(18)-Au(5)	99.5
S(3)-Au(18)-Au(13)#1	84.6
S(3)-Au(18)-Au(17)	130.6
Au(2)-Au(19)-Au(3)	55.3
Au(2)-Au(19)-Au(15)#1	52.7
Au(2)-Au(19)-Au(20)	85.0
Au(3)-Au(19)-Au(20)	115.2
Au(15)#1-Au(19)-Au(3)	55.2
Au(15)#1-Au(19)-Au(20)	60.0
S(5)-Au(19)-Au(2)	101.8
S(5)-Au(19)-Au(3)	47.5
S(5)-Au(19)-Au(15)#1	89.4
S(5)-Au(19)-Au(20)	135.6
S(6)-Au(19)-Au(2)	80.6
S(6)-Au(19)-Au(3)	134.9
S(6)-Au(19)-Au(15)#1	92.4
S(6)-Au(19)-Au(20)	44.7
S(6)-Au(19)-S(5)	177.6
Au(15)#1-Au(20)-Au(19)	57.9
Au(15)#1-Au(20)-Au(21)	54.8
Au(16)#1-Au(20)-Au(15)#1	51.4
Au(16)#1-Au(20)-Au(19)	84.8
Au(16)#1-Au(20)-Au(21)	55.6
Au(21)-Au(20)-Au(19)	112.6
S(6)-Au(20)-Au(15)#1	89.7
S(6)-Au(20)-Au(16)#1	82.1
S(6)-Au(20)-Au(19)	43.4

S(6)-Au(20)-Au(21)	135.6
S(7)-Au(20)-Au(15)#1	92.7
S(7)-Au(20)-Au(16)#1	99.4
S(7)-Au(20)-Au(19)	138.4
S(7)-Au(20)-Au(21)	46.4
S(7)-Au(20)-S(6)	177.6
Au(5)#1-Au(21)-Au(9)#1	62.2
Au(5)#1-Au(21)-Au(10)#1	89.6
Au(5)#1-Au(21)-Au(13)	60.5
Au(5)#1-Au(21)-Au(15)#1	123.9
Au(5)#1-Au(21)-Au(16)#1	122.4
Au(5)#1-Au(21)-Au(17)#1	91.2
Au(5)#1-Au(21)-Au(20)	173.8
Au(9)#1-Au(21)-Au(10)#1	65.6
Au(9)#1-Au(21)-Au(15)#1	61.6
Au(9)#1-Au(21)-Au(16)#1	88.2
Au(9)#1-Au(21)-Au(17)#1	126.1
Au(9)#1-Au(21)-Au(20)	124.0
Au(10)#1-Au(21)-Au(17)#1	166.7
Au(10)#1-Au(21)-Au(20)	93.2
Au(13)-Au(21)-Au(9)#1	62.1
Au(13)-Au(21)-Au(10)#1	127.2
Au(13)-Au(21)-Au(15)#1	92.4
Au(13)-Au(21)-Au(16)#1	62.0
Au(13)-Au(21)-Au(17)#1	64.0
Au(13)-Au(21)-Au(20)	121.2
Au(15)#1-Au(21)-Au(10)#1	68.2
Au(15)#1-Au(21)-Au(17)#1	121.6
Au(15)#1-Au(21)-Au(20)	62.3
Au(16)#1-Au(21)-Au(10)#1	123.3
Au(16)#1-Au(21)-Au(15)#1	55.2
Au(16)#1-Au(21)-Au(17)#1	66.8
Au(16)#1-Au(21)-Au(20)	60.1
Au(17)#1-Au(21)-Au(20)	84.8
S(7)-Au(21)-Au(5)#1	130.8
S(7)-Au(21)-Au(9)#1	146.1
S(7)-Au(21)-Au(10)#1	82.2
S(7)-Au(21)-Au(13)	150.5

S(7)-Au(21)-Au(15)#1	97.7
S(7)-Au(21)-Au(16)#1	101.9
S(7)-Au(21)-Au(17)#1	87.3
S(7)-Au(21)-Au(20)	44.4
Au(1)-Au(22)-Au(6)	62.0
Au(1)-Au(22)-Au(7)	60.9
Au(1)-Au(22)-Au(23)	73.0
Au(1)-Au(22)-Au(24)	74.3
Au(1)-Au(22)-Au(26)	141.2
Au(6)-Au(22)-Au(7)	59.3
Au(6)-Au(22)-Au(23)	134.9
Au(6)-Au(22)-Au(24)	98.3
Au(6)-Au(22)-Au(26)	90.3
Au(7)-Au(22)-Au(23)	96.9
Au(7)-Au(22)-Au(24)	135.2
Au(7)-Au(22)-Au(26)	82.0
Au(23)-Au(22)-Au(24)	71.1
Au(23)-Au(22)-Au(26)	126.3
Au(26)-Au(22)-Au(24)	140.4
S(15)-Au(22)-Au(1)	169.1
S(15)-Au(22)-Au(6)	126.6
S(15)-Au(22)-Au(7)	128.0
S(15)-Au(22)-Au(23)	98.4
S(15)-Au(22)-Au(24)	96.7
S(15)-Au(22)-Au(26)	49.5
Au(2)-Au(23)-Au(1)	54.1
Au(3)-Au(23)-Au(1)	50.6
Au(3)-Au(23)-Au(2)	53.9
Au(22)-Au(23)-Au(1)	51.5
Au(22)-Au(23)-Au(2)	83.9
Au(22)-Au(23)-Au(3)	102.0
S(4)-Au(23)-Au(1)	96.8
S(4)-Au(23)-Au(2)	141.6
S(4)-Au(23)-Au(3)	88.8
S(4)-Au(23)-Au(22)	96.9
S(8)-Au(23)-Au(1)	90.2
S(8)-Au(23)-Au(2)	46.4
S(8)-Au(23)-Au(3)	98.7

S(8)-Au(23)-Au(22)	84.3
S(8)-Au(23)-S(4)	171.9
Au(4)-Au(24)-Au(5)	57.0
Au(22)-Au(24)-Au(4)	98.7
Au(22)-Au(24)-Au(5)	80.4
S(4)-Au(24)-Au(4)	85.8
S(4)-Au(24)-Au(5)	140.1
S(4)-Au(24)-Au(22)	92.6
S(14)-Au(24)-Au(4)	99.1
S(14)-Au(24)-Au(5)	48.5
S(14)-Au(24)-Au(22)	96.4
S(14)-Au(24)-S(4)	169.0
S(11)-Au(25)-Au(7)	93.3
S(16)-Au(25)-Au(7)	93.7
S(16)-Au(25)-S(11)	172.3
S(15)-Au(26)-Au(22)	51.6
S(15)-Au(26)-S(16)	177.6
S(16)-Au(26)-Au(22)	127.4
Au(17)-S(1)-Au(16)	92.5
C(1)-S(1)-Au(16)	114.1
C(1)-S(1)-Au(17)	99.8
Au(18)-S(2)-Au(17)	86.3
C(9)-S(2)-Au(17)	95.2
C(9)-S(2)-Au(18)	91.8
Au(18)-S(3)-Au(4)	89.0
C(17)-S(3)-Au(4)	113.4
C(17)-S(3)-Au(18)	111.6
Au(23)-S(4)-Au(24)	95.1
C(25)-S(4)-Au(23)	104.0
C(25)-S(4)-Au(24)	104.4
Au(19)-S(5)-Au(3)	87.1
C(33)-S(5)-Au(3)	133.0
C(33)-S(5)-Au(19)	92.2
Au(19)-S(6)-Au(20)	91.9
C(41)-S(6)-Au(19)	119.5
C(41)-S(6)-Au(20)	108.2
Au(20)-S(7)-Au(21)	89.1
C(49)-S(7)-Au(20)	146.9

C(49)-S(7)-Au(21)	109.9
Au(23)-S(8)-Au(2)	90.5
C(57)-S(8)-Au(2)	114.5
C(57)-S(8)-Au(23)	100.6
Au(12)-S(9)-Au(7)	81.6
C(65)-S(9)-Au(7)	115.0
C(65)-S(9)-Au(12)	108.0
Au(12)-S(10)-Au(13)	95.7
C(73)-S(10)-Au(12)	100.3
C(73)-S(10)-Au(13)	113.1
Au(25)-S(11)-Au(11)	100.3
C(81)-S(11)-Au(11)	112.4
C(81)-S(11)-Au(25)	107.3
Au(10)-S(12)-Au(15)	92.0
C(89)-S(12)-Au(10)	104.5
C(89)-S(12)-Au(15)	114.2
Au(10)-S(13)-Au(6)	82.6
C(97)-S(13)-Au(6)	138.3
C(97)-S(13)-Au(10)	91.2
Au(24)-S(14)-Au(5)	85.0
C(105)-S(14)-Au(5)	121.1
C(105)-S(14)-Au(24)	106.8
Au(26)-S(15)-Au(22)	78.9
C(113)-S(15)-Au(22)	115.3
C(113)-S(15)-Au(26)	110.6
Au(25)-S(16)-Au(26)	102.2
C(121)-S(16)-Au(25)	103.7
C(121)-S(16)-Au(26)	147.4
S(1)-C(1)-H(1A)	109.0
S(1)-C(1)-H(1B)	109.0
H(1A)-C(1)-H(1B)	107.8
C(2)-C(1)-S(1)	113.0
C(2)-C(1)-H(1A)	109.0
C(2)-C(1)-H(1B)	109.0
C(1)-C(2)-H(2A)	107.3
C(1)-C(2)-H(2B)	107.3
C(1)-C(2)-C(3)	120.3
H(2A)-C(2)-H(2B)	106.9

C(3)-C(2)-H(2A)	107.3
C(3)-C(2)-H(2B)	107.3
C(8)-C(3)-C(2)	113.4
C(8)-C(3)-C(4)	120.0
C(4)-C(3)-C(2)	126.2
C(3)-C(8)-H(8)	120.0
C(7)-C(8)-C(3)	120.0
C(7)-C(8)-H(8)	120.0
C(8)-C(7)-H(7)	120.0
C(8)-C(7)-C(6)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-C(7)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(5)-H(5)	120.0
C(6)-C(5)-C(4)	120.0
C(4)-C(5)-H(5)	120.0
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-C(3)	120.0
C(5)-C(4)-H(4)	120.0
S(2)-C(9)-H(9A)	101.7
S(2)-C(9)-H(9B)	101.7
H(9A)-C(9)-H(9B)	104.7
C(10)-C(9)-S(2)	141.4
C(10)-C(9)-H(9A)	101.7
C(10)-C(9)-H(9B)	101.7
C(11)-C(10)-C(9)	86.8
C(13)-C(12)-C(11)	120.0
C(12)-C(13)-C(14)	120.0
C(15)-C(14)-C(13)	120.0
C(14)-C(15)-C(16)	120.0
C(15)-C(16)-C(11)	120.0
C(12)-C(11)-C(10)	121.5
C(16)-C(11)-C(10)	118.4
C(16)-C(11)-C(12)	120.0
S(3)-C(17)-H(17A)	108.2
S(3)-C(17)-H(17B)	108.2
H(17A)-C(17)-H(17B)	107.3

C(18)-C(17)-S(3)	116.4
C(18)-C(17)-H(17A)	108.2
C(18)-C(17)-H(17B)	108.2
C(17)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.3
C(19)-C(18)-C(17)	109.2
C(19)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18B)	109.8
C(20)-C(19)-C(18)	122.6
C(20)-C(19)-C(24)	120.0
C(24)-C(19)-C(18)	117.2
C(19)-C(20)-H(20)	120.0
C(19)-C(20)-C(21)	120.0
C(21)-C(20)-H(20)	120.0
C(20)-C(21)-H(21)	120.0
C(20)-C(21)-C(22)	120.0
C(22)-C(21)-H(21)	120.0
C(21)-C(22)-H(22)	120.0
C(23)-C(22)-C(21)	120.0
C(23)-C(22)-H(22)	120.0
C(22)-C(23)-H(23)	120.0
C(22)-C(23)-C(24)	120.0
C(24)-C(23)-H(23)	120.0
C(19)-C(24)-H(24)	120.0
C(23)-C(24)-C(19)	120.0
C(23)-C(24)-H(24)	120.0
C(26)-C(25)-S(4)	113.7
C(27)-C(26)-C(25)	104.3
C(32)-C(27)-C(26)	105.5
C(32)-C(27)-C(28)	120.0
C(28)-C(27)-C(26)	133.7
C(27)-C(32)-H(32)	120.0
C(27)-C(32)-C(31)	120.0
C(31)-C(32)-H(32)	120.0
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-C(32)	120.0
C(30)-C(31)-H(31)	120.0

C(31)-C(30)-H(30)	120.0
C(29)-C(30)-C(31)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(29)-H(29)	120.0
C(28)-C(29)-C(30)	120.0
C(28)-C(29)-H(29)	120.0
C(27)-C(28)-H(28)	120.0
C(29)-C(28)-C(27)	120.0
C(29)-C(28)-H(28)	120.0
S(5)-C(33)-H(33A)	107.1
S(5)-C(33)-H(33B)	107.1
H(33A)-C(33)-H(33B)	106.8
C(34)-C(33)-S(5)	120.8
C(34)-C(33)-H(33A)	107.1
C(34)-C(33)-H(33B)	107.1
C(35)-C(34)-C(33)	115.3
C(40)-C(35)-C(34)	130.1
C(40)-C(35)-C(36)	120.0
C(36)-C(35)-C(34)	109.8
C(39)-C(40)-C(35)	120.0
C(40)-C(39)-C(38)	120.0
C(39)-C(38)-C(37)	120.0
C(36)-C(37)-C(38)	120.0
C(37)-C(36)-C(35)	120.0
S(6)-C(41)-H(41A)	111.8
S(6)-C(41)-H(41B)	111.8
H(41A)-C(41)-H(41B)	109.5
C(42)-C(41)-S(6)	100.0
C(42)-C(41)-H(41A)	111.8
C(42)-C(41)-H(41B)	111.8
C(41)-C(42)-C(43)	106.6
C(47)-C(48)-C(43)	120.0
C(48)-C(47)-C(46)	120.0
C(45)-C(46)-C(47)	120.0
C(46)-C(45)-C(44)	120.0
C(45)-C(44)-C(43)	120.0
C(48)-C(43)-C(42)	104.5
C(44)-C(43)-C(42)	126.9

C(44)-C(43)-C(48)	120.0
S(7)-C(49)-H(49A)	112.1
S(7)-C(49)-H(49B)	112.1
H(49A)-C(49)-H(49B)	109.7
C(50)-C(49)-S(7)	98.6
C(50)-C(49)-H(49A)	112.1
C(50)-C(49)-H(49B)	112.1
C(49)-C(50)-H(50A)	110.6
C(49)-C(50)-H(50B)	110.6
C(49)-C(50)-C(51)	105.8
H(50A)-C(50)-H(50B)	108.7
C(51)-C(50)-H(50A)	110.6
C(51)-C(50)-H(50B)	110.6
C(53)-C(52)-H(52)	120.0
C(53)-C(52)-C(51)	120.0
C(51)-C(52)-H(52)	120.0
C(52)-C(53)-H(53)	120.0
C(52)-C(53)-C(54)	120.0
C(54)-C(53)-H(53)	120.0
C(53)-C(54)-H(54)	120.0
C(53)-C(54)-C(55)	120.0
C(55)-C(54)-H(54)	120.0
C(54)-C(55)-H(55)	120.0
C(56)-C(55)-C(54)	120.0
C(56)-C(55)-H(55)	120.0
C(55)-C(56)-H(56)	120.0
C(51)-C(56)-C(55)	120.0
C(51)-C(56)-H(56)	120.0
C(52)-C(51)-C(50)	135.4
C(56)-C(51)-C(50)	104.6
C(56)-C(51)-C(52)	120.0
S(8)-C(57)-H(57A)	108.4
S(8)-C(57)-H(57B)	108.4
H(57A)-C(57)-H(57B)	107.4
C(58)-C(57)-S(8)	115.6
C(58)-C(57)-H(57A)	108.4
C(58)-C(57)-H(57B)	108.4
C(57)-C(58)-H(58A)	109.2

C(57)-C(58)-H(58B)	109.2
C(57)-C(58)-C(59)	112.1
H(58A)-C(58)-H(58B)	107.9
C(59)-C(58)-H(58A)	109.2
C(59)-C(58)-H(58B)	109.2
C(60)-C(59)-C(58)	121.3
C(60)-C(59)-C(64)	120.0
C(64)-C(59)-C(58)	118.7
C(59)-C(60)-H(60)	120.0
C(61)-C(60)-C(59)	120.0
C(61)-C(60)-H(60)	120.0
C(60)-C(61)-H(61)	120.0
C(60)-C(61)-C(62)	120.0
C(62)-C(61)-H(61)	120.0
C(61)-C(62)-H(62)	120.0
C(61)-C(62)-C(63)	120.0
C(63)-C(62)-H(62)	120.0
C(62)-C(63)-H(63)	120.0
C(64)-C(63)-C(62)	120.0
C(64)-C(63)-H(63)	120.0
C(59)-C(64)-H(64)	120.0
C(63)-C(64)-C(59)	120.0
C(63)-C(64)-H(64)	120.0
S(9)-C(65)-H(65A)	109.1
S(9)-C(65)-H(65B)	109.1
H(65A)-C(65)-H(65B)	107.9
C(66)-C(65)-S(9)	112.3
C(66)-C(65)-H(65A)	109.1
C(66)-C(65)-H(65B)	109.1
C(65)-C(66)-C(67)	119.2
C(72)-C(67)-C(66)	119.1
C(72)-C(67)-C(68)	120.0
C(68)-C(67)-C(66)	120.5
C(67)-C(72)-H(72)	120.0
C(71)-C(72)-C(67)	120.0
C(71)-C(72)-H(72)	120.0
C(72)-C(71)-H(71)	120.0
C(70)-C(71)-C(72)	120.0

C(70)-C(71)-H(71)	120.0
C(71)-C(70)-H(70)	120.0
C(71)-C(70)-C(69)	120.0
C(69)-C(70)-H(70)	120.0
C(70)-C(69)-H(69)	120.0
C(68)-C(69)-C(70)	120.0
C(68)-C(69)-H(69)	120.0
C(67)-C(68)-H(68)	120.0
C(69)-C(68)-C(67)	120.0
C(69)-C(68)-H(68)	120.0
S(10)-C(73)-H(73A)	109.0
S(10)-C(73)-H(73B)	109.0
H(73A)-C(73)-H(73B)	107.8
C(74)-C(73)-S(10)	112.8
C(74)-C(73)-H(73A)	109.0
C(74)-C(73)-H(73B)	109.0
C(75)-C(74)-C(73)	113.9
C(76)-C(75)-C(74)	122.7
C(76)-C(75)-C(80)	120.0
C(80)-C(75)-C(74)	117.3
C(75)-C(76)-H(76)	120.0
C(75)-C(76)-C(77)	120.0
C(77)-C(76)-H(76)	120.0
C(76)-C(77)-H(77)	120.0
C(78)-C(77)-C(76)	120.0
C(78)-C(77)-H(77)	120.0
C(77)-C(78)-H(78)	120.0
C(79)-C(78)-C(77)	120.0
C(79)-C(78)-H(78)	120.0
C(78)-C(79)-H(79)	120.0
C(78)-C(79)-C(80)	120.0
C(80)-C(79)-H(79)	120.0
C(75)-C(80)-H(80)	120.0
C(79)-C(80)-C(75)	120.0
C(79)-C(80)-H(80)	120.0
S(11)-C(81)-H(81A)	108.9
S(11)-C(81)-H(81B)	108.9
H(81A)-C(81)-H(81B)	107.7

C(82)-C(81)-S(11)	113.6
C(82)-C(81)-H(81A)	108.9
C(82)-C(81)-H(81B)	108.9
C(81)-C(82)-H(82A)	109.8
C(81)-C(82)-H(82B)	109.8
C(81)-C(82)-C(83)	109.5
H(82A)-C(82)-H(82B)	108.2
C(83)-C(82)-H(82A)	109.8
C(83)-C(82)-H(82B)	109.8
C(88)-C(83)-C(82)	119.9
C(88)-C(83)-C(84)	120.0
C(84)-C(83)-C(82)	120.1
C(83)-C(88)-H(88)	120.0
C(87)-C(88)-C(83)	120.0
C(87)-C(88)-H(88)	120.0
C(88)-C(87)-H(87)	120.0
C(86)-C(87)-C(88)	120.0
C(86)-C(87)-H(87)	120.0
C(87)-C(86)-H(86)	120.0
C(85)-C(86)-C(87)	120.0
C(85)-C(86)-H(86)	120.0
C(86)-C(85)-H(85)	120.0
C(86)-C(85)-C(84)	120.0
C(84)-C(85)-H(85)	120.0
C(83)-C(84)-H(84)	120.0
C(85)-C(84)-C(83)	120.0
C(85)-C(84)-H(84)	120.0
S(12)-C(89)-H(89A)	107.5
S(12)-C(89)-H(89B)	107.5
H(89A)-C(89)-H(89B)	107.0
C(90)-C(89)-S(12)	119.1
C(90)-C(89)-H(89A)	107.5
C(90)-C(89)-H(89B)	107.5
C(89)-C(90)-H(90A)	107.8
C(89)-C(90)-H(90B)	107.8
H(90A)-C(90)-H(90B)	107.1
C(91)-C(90)-C(89)	118.2
C(91)-C(90)-H(90A)	107.8

C(91)-C(90)-H(90B)	107.8
C(92)-C(91)-C(90)	103.2
C(92)-C(91)-C(96)	120.0
C(96)-C(91)-C(90)	136.8
C(91)-C(92)-H(92)	120.0
C(93)-C(92)-C(91)	120.0
C(93)-C(92)-H(92)	120.0
C(92)-C(93)-H(93)	120.0
C(92)-C(93)-C(94)	120.0
C(94)-C(93)-H(93)	120.0
C(93)-C(94)-H(94)	120.0
C(95)-C(94)-C(93)	120.0
C(95)-C(94)-H(94)	120.0
C(94)-C(95)-H(95)	120.0
C(96)-C(95)-C(94)	120.0
C(96)-C(95)-H(95)	120.0
C(91)-C(96)-H(96)	120.0
C(95)-C(96)-C(91)	120.0
C(95)-C(96)-H(96)	120.0
C(98)-C(97)-S(13)	176.4
C(97)-C(98)-C(99)	166.9
C(100)-C(99)-C(98)	138.1
C(100)-C(99)-C(104)	120.0
C(104)-C(99)-C(98)	97.6
C(99)-C(100)-C(101)	120.0
C(102)-C(101)-C(100)	120.0
C(103)-C(102)-C(101)	120.0
C(104)-C(103)-C(102)	120.0
C(103)-C(104)-C(99)	120.0
S(14)-C(105)-H(10A)	101.2
S(14)-C(105)-H(10B)	101.2
H(10A)-C(105)-H(10B)	104.5
C(106)-C(105)-S(14)	143.1
C(106)-C(105)-H(10A)	101.2
C(106)-C(105)-H(10B)	101.2
C(105)-C(106)-C(107)	105.9
C(108)-C(107)-C(106)	104.8
C(108)-C(107)-C(112)	120.0

C(112)-C(107)-C(106)	131.5
C(107)-C(108)-H(108)	120.0
C(109)-C(108)-C(107)	120.0
C(109)-C(108)-H(108)	120.0
C(108)-C(109)-H(109)	120.0
C(108)-C(109)-C(110)	120.0
C(110)-C(109)-H(109)	120.0
C(109)-C(110)-H(110)	120.0
C(111)-C(110)-C(109)	120.0
C(111)-C(110)-H(110)	120.0
C(110)-C(111)-H(111)	120.0
C(110)-C(111)-C(112)	120.0
C(112)-C(111)-H(111)	120.0
C(107)-C(112)-H(112)	120.0
C(111)-C(112)-C(107)	120.0
C(111)-C(112)-H(112)	120.0
S(15)-C(113)-H(11A)	113.3
S(15)-C(113)-H(11B)	113.3
H(11A)-C(113)-H(11B)	110.7
C(114)-C(113)-S(15)	91.7
C(114)-C(113)-H(11A)	113.3
C(114)-C(113)-H(11B)	113.3
C(113)-C(114)-H(11C)	110.3
C(113)-C(114)-H(11D)	110.3
H(11C)-C(114)-H(11D)	108.6
C(115)-C(114)-C(113)	107.1
C(115)-C(114)-H(11C)	110.3
C(115)-C(114)-H(11D)	110.3
C(120)-C(115)-C(114)	106.8
C(120)-C(115)-C(116)	120.0
C(116)-C(115)-C(114)	133.2
C(119)-C(120)-C(115)	120.0
C(118)-C(119)-C(120)	120.0
C(117)-C(118)-C(119)	120.0
C(118)-C(117)-C(116)	120.0
C(117)-C(116)-C(115)	120.0
S(16)-C(121)-H(12A)	112.3
S(16)-C(121)-H(12B)	112.3

H(12A)-C(121)-H(12B)	109.9
C(122)-C(121)-S(16)	97.4
C(122)-C(121)-H(12A)	112.3
C(122)-C(121)-H(12B)	112.3
C(121)-C(122)-H(12C)	112.7
C(121)-C(122)-H(12D)	112.7
H(12C)-C(122)-H(12D)	110.2
C(123)-C(122)-C(121)	95.2
C(123)-C(122)-H(12C)	112.7
C(123)-C(122)-H(12D)	112.7
C(128)-C(123)-C(122)	119.5
C(128)-C(123)-C(124)	120.0
C(124)-C(123)-C(122)	120.5
C(127)-C(128)-C(123)	120.0
C(126)-C(127)-C(128)	120.0
C(125)-C(126)-C(127)	120.0
C(126)-C(125)-C(124)	120.0
C(125)-C(124)-C(123)	120.0

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for $Au_{52}(PET)_{32}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	46(1)	45(1)	44(1)	19(1)	3(1)	6(1)
Au(2)	52(1)	46(1)	58(1)	21(1)	7(1)	4(1)
Au(3)	58(1)	48(1)	61(1)	21(1)	12(1)	10(1)
Au(4)	53(1)	47(1)	54(1)	17(1)	6(1)	6(1)
Au(5)	57(1)	63(1)	46(1)	25(1)	5(1)	8(1)
Au(6)	64(1)	65(1)	52(1)	28(1)	5(1)	8(1)
Au(7)	53(1)	52(1)	59(1)	22(1)	7(1)	5(1)
Au(8)	42(1)	38(1)	41(1)	19(1)	3(1)	5(1)
Au(9)	41(1)	44(1)	40(1)	23(1)	5(1)	7(1)
Au(10)	74(1)	77(1)	85(1)	47(1)	19(1)	12(1)
Au(11)	51(1)	52(1)	54(1)	27(1)	10(1)	10(1)
Au(12)	62(1)	50(1)	64(1)	22(1)	12(1)	6(1)
Au(13)	47(1)	44(1)	48(1)	20(1)	5(1)	6(1)
Au(14)	42(1)	40(1)	40(1)	21(1)	7(1)	7(1)
Au(15)	58(1)	46(1)	51(1)	26(1)	9(1)	10(1)
Au(16)	54(1)	50(1)	58(1)	22(1)	12(1)	5(1)
Au(17)	80(1)	65(1)	70(1)	29(1)	19(1)	15(1)
Au(18)	70(1)	72(1)	66(1)	21(1)	7(1)	11(1)
Au(19)	83(1)	61(1)	100(1)	41(1)	10(1)	4(1)
Au(20)	84(1)	69(1)	97(1)	45(1)	26(1)	16(1)
Au(21)	65(1)	58(1)	55(1)	30(1)	11(1)	10(1)
Au(22)	71(1)	67(1)	56(1)	16(1)	-1(1)	7(1)
Au(23)	65(1)	59(1)	74(1)	13(1)	4(1)	9(1)
Au(24)	71(1)	80(1)	65(1)	8(1)	-3(1)	14(1)
Au(25)	74(1)	84(1)	94(1)	47(1)	-1(1)	13(1)
Au(26)	90(2)	108(2)	94(2)	34(1)	-13(1)	18(1)
S(1)	85(5)	85(5)	84(5)	40(4)	22(4)	7(4)
S(2)	118(7)	122(6)	116(6)	62(5)	15(5)	30(5)
S(3)	78(5)	75(5)	72(5)	32(4)	9(4)	12(4)
S(4)	103(6)	104(6)	102(6)	39(5)	16(5)	21(5)
S(5)	126(7)	104(6)	128(6)	75(5)	25(5)	27(5)
S(6)	115(7)	106(6)	123(6)	62(5)	27(5)	9(5)
S(7)	174(8)	159(8)	155(8)	94(7)	32(6)	5(6)

S(8)	71(5)	76(5)	87(5)	32(4)	13(4)	6(4)
S(9)	60(5)	66(4)	70(4)	29(4)	8(4)	14(4)
S(10)	60(4)	63(4)	66(4)	30(3)	8(4)	8(4)
S(11)	80(5)	79(5)	85(5)	50(4)	4(4)	21(4)
S(12)	80(5)	83(5)	88(5)	52(4)	20(4)	7(4)
S(13)	119(7)	122(6)	110(6)	77(5)	28(5)	13(5)
S(14)	115(7)	121(6)	103(6)	46(5)	21(5)	18(5)
S(15)	140(8)	148(7)	137(7)	67(6)	17(6)	27(6)
S(16)	138(8)	141(7)	150(7)	79(6)	18(6)	28(6)
C(1)	93(5)	92(5)	93(5)	42(3)	17(4)	10(4)
C(2)	100(5)	100(5)	101(5)	45(3)	16(3)	13(3)
C(3)	106(5)	106(5)	106(5)	48(3)	17(3)	14(3)
C(8)	109(6)	109(6)	109(6)	50(4)	17(3)	14(3)
C(7)	111(6)	111(6)	112(6)	51(4)	17(3)	15(3)
C(6)	112(6)	112(6)	112(6)	51(4)	17(3)	15(3)
C(5)	111(6)	111(6)	111(6)	51(4)	17(3)	15(3)
C(4)	109(6)	109(6)	109(6)	50(4)	17(3)	15(3)
C(9)	128(6)	130(6)	128(6)	60(4)	18(4)	24(4)
C(10)	137(6)	138(6)	137(6)	63(4)	21(3)	22(3)
C(12)	148(7)	148(7)	148(7)	67(4)	22(3)	21(3)
C(13)	150(7)	150(7)	150(7)	68(4)	22(4)	21(4)
C(14)	150(7)	151(7)	151(7)	68(4)	22(4)	22(4)
C(15)	150(7)	150(7)	150(7)	68(4)	22(4)	22(4)
C(16)	148(7)	148(7)	147(7)	67(4)	22(3)	21(3)
C(11)	145(6)	145(6)	144(6)	66(4)	22(3)	22(3)
C(17)	85(5)	84(5)	83(5)	37(3)	11(3)	13(3)
C(18)	94(5)	93(5)	93(5)	41(3)	14(3)	14(3)
C(19)	101(5)	101(5)	101(5)	45(3)	16(3)	15(3)
C(20)	104(6)	104(5)	104(5)	46(4)	16(3)	14(3)
C(21)	106(6)	107(6)	106(6)	47(4)	16(3)	15(3)
C(22)	107(6)	107(6)	107(6)	47(4)	17(3)	15(3)
C(23)	107(6)	107(6)	107(6)	47(4)	17(3)	15(3)
C(24)	104(6)	105(5)	104(5)	46(4)	16(3)	15(3)
C(25)	110(5)	111(5)	110(5)	48(4)	17(4)	19(4)
C(26)	119(6)	119(6)	119(6)	53(4)	18(3)	18(3)
C(27)	126(6)	126(6)	126(6)	56(3)	19(3)	19(3)
C(32)	130(6)	130(6)	130(6)	58(4)	19(3)	19(3)
C(31)	132(6)	132(6)	131(6)	59(4)	19(3)	19(3)

C(30)	132(7)	132(6)	132(7)	59(4)	19(4)	19(3)
C(29)	131(6)	131(6)	131(6)	59(4)	19(3)	19(3)
C(28)	129(6)	129(6)	129(6)	58(4)	19(3)	19(3)
C(33)	135(6)	129(6)	138(6)	65(4)	22(4)	23(4)
C(34)	145(6)	143(6)	147(6)	66(4)	21(3)	23(3)
C(35)	153(6)	152(6)	154(6)	69(4)	22(3)	23(3)
C(40)	157(7)	156(7)	157(7)	71(4)	23(3)	23(3)
C(39)	159(7)	158(7)	158(7)	72(4)	23(4)	24(4)
C(38)	159(7)	159(7)	159(7)	72(4)	23(4)	24(4)
C(37)	158(7)	158(7)	159(7)	72(4)	23(4)	23(4)
C(36)	157(7)	156(7)	157(7)	71(4)	22(3)	23(3)
C(41)	124(6)	121(6)	127(6)	59(4)	23(4)	15(4)
C(42)	131(6)	131(6)	132(6)	60(4)	21(3)	18(3)
C(48)	139(7)	139(6)	140(6)	63(4)	20(3)	21(3)
C(47)	140(7)	141(7)	140(7)	64(4)	21(4)	22(3)
C(46)	141(7)	142(7)	141(7)	64(4)	21(4)	21(4)
C(45)	140(7)	141(7)	140(7)	64(4)	21(4)	21(3)
C(44)	139(7)	139(6)	139(6)	63(4)	21(3)	21(3)
C(43)	137(6)	137(6)	137(6)	62(4)	21(3)	20(3)
C(49)	173(8)	168(7)	167(7)	83(5)	28(4)	17(4)
C(50)	175(8)	173(7)	173(8)	81(4)	27(4)	22(4)
C(52)	178(8)	178(8)	178(8)	81(4)	26(4)	25(4)
C(53)	178(8)	178(8)	178(8)	82(4)	26(4)	26(4)
C(54)	178(8)	179(8)	178(8)	81(5)	27(4)	26(4)
C(55)	178(8)	179(8)	178(8)	82(4)	27(4)	26(4)
C(56)	178(8)	178(8)	177(8)	81(4)	27(4)	26(4)
C(51)	177(8)	177(8)	176(8)	81(4)	27(3)	25(3)
C(57)	85(5)	86(5)	91(5)	39(3)	14(4)	10(3)
C(58)	95(5)	96(5)	99(5)	43(3)	16(3)	13(3)
C(59)	104(5)	104(5)	107(5)	47(3)	16(3)	15(3)
C(60)	108(6)	108(6)	110(6)	49(4)	18(3)	15(3)
C(61)	111(6)	111(6)	112(6)	50(4)	18(3)	16(3)
C(62)	112(6)	113(6)	113(6)	50(4)	17(3)	17(3)
C(63)	111(6)	112(6)	113(6)	50(4)	17(3)	16(3)
C(64)	108(6)	109(6)	111(6)	48(4)	16(3)	16(3)
C(65)	68(4)	70(4)	71(4)	31(3)	10(3)	12(3)
C(66)	73(5)	74(4)	75(4)	32(3)	12(3)	11(3)
C(67)	78(5)	79(4)	79(4)	35(3)	13(3)	12(3)

C(72)	82(5)	82(5)	82(5)	36(3)	14(3)	12(3)
C(71)	83(5)	83(5)	83(5)	37(3)	13(3)	11(3)
C(70)	82(5)	83(5)	83(5)	37(3)	14(3)	11(3)
C(69)	81(5)	82(5)	82(5)	37(3)	13(3)	11(3)
C(68)	80(5)	81(5)	80(5)	36(3)	13(3)	12(3)
C(73)	66(4)	66(4)	68(4)	32(3)	11(3)	7(3)
C(74)	71(4)	71(4)	73(4)	32(3)	12(3)	10(3)
C(75)	76(4)	76(4)	78(4)	35(3)	12(3)	11(3)
C(76)	78(5)	79(5)	79(5)	35(3)	12(3)	12(3)
C(77)	80(5)	80(5)	81(5)	37(3)	12(3)	11(3)
C(78)	81(5)	83(5)	82(5)	36(3)	13(3)	12(3)
C(79)	80(5)	82(5)	82(5)	36(3)	13(3)	11(3)
C(80)	78(5)	80(5)	79(5)	36(3)	13(3)	11(3)
C(81)	85(5)	84(5)	87(5)	42(3)	9(3)	16(3)
C(82)	88(5)	88(5)	89(5)	42(3)	11(3)	14(3)
C(83)	91(5)	91(5)	92(5)	42(3)	14(3)	14(3)
C(88)	93(5)	93(5)	94(5)	43(3)	14(3)	14(3)
C(87)	95(6)	95(5)	96(5)	43(4)	14(3)	14(3)
C(86)	96(6)	96(6)	96(6)	44(4)	14(3)	14(3)
C(85)	95(6)	96(5)	96(5)	43(4)	15(3)	14(3)
C(84)	93(5)	94(5)	94(5)	43(3)	14(3)	14(3)
C(89)	89(5)	91(5)	92(5)	46(3)	16(4)	11(3)
C(90)	97(5)	98(5)	98(5)	46(3)	16(3)	13(3)
C(91)	103(5)	102(5)	104(5)	48(3)	15(3)	14(3)
C(92)	106(6)	106(6)	106(6)	49(4)	16(3)	14(3)
C(93)	108(6)	108(6)	108(6)	49(4)	16(3)	15(3)
C(94)	108(6)	108(6)	108(6)	50(4)	15(3)	16(3)
C(95)	107(6)	107(6)	107(6)	50(4)	15(3)	15(3)
C(96)	106(6)	105(6)	106(6)	49(4)	15(3)	15(3)
C(97)	130(6)	133(6)	128(6)	65(4)	23(4)	17(4)
C(98)	138(6)	140(6)	138(6)	65(4)	21(3)	19(3)
C(99)	146(6)	146(6)	147(6)	67(4)	22(3)	21(3)
C(100)	149(7)	150(7)	150(7)	68(4)	22(3)	21(3)
C(101)	151(7)	152(7)	152(7)	69(4)	23(4)	22(4)
C(102)	152(7)	152(7)	152(7)	69(4)	22(4)	22(4)
C(103)	151(7)	152(7)	152(7)	69(4)	22(4)	22(4)
C(104)	149(7)	150(7)	150(7)	68(4)	22(3)	22(3)
C(105)	122(6)	125(6)	118(6)	54(4)	20(4)	18(4)

C(106)	130(6)	131(6)	129(6)	58(4)	20(3)	19(3)
C(107)	136(6)	137(6)	137(6)	61(4)	21(3)	20(3)
C(108)	139(7)	140(7)	139(7)	62(4)	22(3)	20(3)
C(109)	140(7)	141(7)	141(7)	63(4)	22(4)	21(4)
C(110)	141(7)	141(7)	142(7)	64(4)	21(4)	21(4)
C(111)	140(7)	141(7)	142(7)	63(4)	21(4)	21(4)
C(112)	139(7)	140(7)	140(7)	63(4)	21(3)	21(3)
C(113)	148(7)	152(7)	148(7)	69(4)	20(4)	24(4)
C(114)	157(7)	158(7)	157(7)	72(4)	23(4)	24(4)
C(115)	163(7)	164(7)	164(7)	74(4)	24(3)	24(3)
C(120)	166(7)	167(7)	167(7)	75(4)	25(4)	24(3)
C(119)	168(8)	168(8)	169(8)	76(4)	25(4)	25(4)
C(118)	169(8)	169(8)	169(8)	76(4)	25(4)	25(4)
C(117)	168(8)	168(8)	168(8)	76(4)	25(4)	25(4)
C(116)	166(7)	166(7)	167(7)	76(4)	25(4)	24(3)
C(121)	151(7)	152(7)	156(7)	73(4)	21(4)	25(4)
C(122)	159(7)	161(7)	161(7)	74(4)	23(4)	24(4)
C(123)	166(7)	167(7)	166(7)	76(4)	24(3)	25(3)
C(128)	169(8)	169(7)	169(7)	77(4)	25(4)	24(4)
C(127)	170(8)	171(8)	171(8)	78(4)	26(4)	25(4)
C(126)	171(8)	171(8)	171(8)	78(4)	26(4)	25(4)
C(125)	170(8)	171(8)	171(8)	78(4)	25(4)	25(4)
C(124)	169(8)	169(7)	169(7)	77(4)	25(4)	25(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $Au_{52}(PET)_{32}$.

	x	y	z	U(eq)
H(1A)	8017	6050	3142	111
H(1B)	8489	6464	3906	111
H(2A)	8877	5179	2788	121
H(2B)	9363	5741	3515	121
H(8)	9823	6977	3744	131
H(7)	10316	7787	3328	134
H(6)	10143	7427	2118	135
H(5)	9477	6256	1324	133
H(4)	8984	5446	1741	131
H(9A)	7068	2765	955	153
H(9B)	7435	3464	892	153
H(17A)	5083	1247	1513	102
H(17B)	5847	1050	1326	102
H(18A)	5923	484	2092	113
H(18B)	5155	684	2283	113
H(20)	4120	-193	1500	126
H(21)	3674	-1375	541	129
H(22)	4413	-2045	-258	129
H(23)	5597	-1532	-98	129
H(24)	6043	-349	860	126
H(32)	2902	884	-529	156
H(31)	2193	175	-1629	159
H(30)	1753	-1100	-2004	159
H(29)	2021	-1668	-1279	158
H(28)	2730	-960	-179	155
H(33A)	3180	502	3017	159
H(33B)	3819	82	3108	159
H(41A)	1410	1962	5694	148
H(41B)	1368	1318	4886	148
H(49A)	4367	4578	8360	201
H(49B)	3519	4557	8315	201
H(50A)	3901	3110	7859	208
H(50B)	3386	3496	8431	208

H(52)	4413	4763	9735	214
H(53)	5403	4719	10434	214
H(54)	6024	3682	9994	214
H(55)	5655	2688	8855	214
H(56)	4665	2732	8155	213
H(57A)	2092	1336	3376	106
H(57B)	1452	1773	3691	106
H(58A)	1494	777	2246	117
H(58B)	905	1328	2469	117
H(60)	83	1157	3310	131
H(61)	-583	252	3513	134
H(62)	-302	-983	3080	136
H(63)	645	-1312	2446	135
H(64)	1311	-407	2243	132
H(65A)	1043	3417	3875	84
H(65B)	1608	3710	4574	84
H(72)	607	2690	4308	99
H(71)	-202	1843	4457	100
H(70)	-1072	2300	5172	100
H(69)	-1134	3603	5737	99
H(68)	-325	4450	5588	97
H(73A)	2265	6229	6745	80
H(73B)	2563	7114	7082	80
H(76)	1126	8039	6985	95
H(77)	156	8177	7592	96
H(78)	-430	7129	7650	99
H(79)	-45	5944	7102	98
H(80)	925	5807	6495	95
H(81A)	2326	7356	4549	101
H(81B)	2476	6930	5017	101
H(82A)	3459	8112	5036	105
H(82B)	3599	7690	5512	105
H(88)	3253	8211	6647	112
H(87)	2714	9110	7522	115
H(86)	1987	9850	7239	115
H(85)	1800	9690	6083	115
H(84)	2338	8791	5209	113
H(89A)	5781	8277	4632	107

H(89B)	5606	7668	3821	107
H(90A)	4448	8116	3866	117
H(90B)	4824	8827	4579	117
H(92)	5466	9674	4704	128
H(93)	5979	10568	4390	130
H(94)	5963	10260	3199	129
H(95)	5434	9059	2320	128
H(96)	4921	8164	2634	127
H(10A)	3654	2930	551	147
H(10B)	3572	3646	1245	147
H(108)	2698	4416	357	168
H(109)	1502	3909	-38	170
H(110)	1168	2595	-701	170
H(111)	2030	1788	-970	170
H(112)	3226	2294	-575	168
H(11A)	1761	1381	1136	179
H(11B)	1206	1941	1540	179
H(11C)	753	2006	537	189
H(11D)	1478	1850	214	189
H(12A)	250	5235	2151	183
H(12B)	372	5626	3006	183
H(12C)	1012	6605	2857	193
H(12D)	1637	6094	2814	193

Table 6. Torsion angles [°] for $Au_{52}(PET)_{32}$.

Au(2)-S(8)-C(57)-C(58)	-173.4
Au(3)-S(5)-C(33)-C(34)	-133.8
Au(4)-S(3)-C(17)-C(18)	-88.3
Au(5)-S(14)-C(105)-C(106)	91.7
Au(7)-S(9)-C(65)-C(66)	166.7
Au(10)-S(12)-C(89)-C(90)	82.9
Au(11)-S(11)-C(81)-C(82)	75.6
Au(12)-S(9)-C(65)-C(66)	77.7
Au(12)-S(10)-C(73)-C(74)	-55.2
Au(13)-S(10)-C(73)-C(74)	-155.9
Au(15)-S(12)-C(89)-C(90)	-178.2
Au(16)-S(1)-C(1)-C(2)	171.3
Au(17)-S(1)-C(1)-C(2)	-91.5
Au(17)-S(2)-C(9)-C(10)	13.3
Au(18)-S(2)-C(9)-C(10)	-73.1
Au(18)-S(3)-C(17)-C(18)	172.9
Au(19)-S(5)-C(33)-C(34)	-45.8
Au(19)-S(6)-C(41)-C(42)	46.8
Au(20)-S(6)-C(41)-C(42)	-56.3
Au(20)-S(7)-C(49)-C(50)	73.6
Au(21)-S(7)-C(49)-C(50)	-164.7
Au(22)-S(15)-C(113)-C(114)	-179.8
Au(23)-S(4)-C(25)-C(26)	149.6
Au(23)-S(8)-C(57)-C(58)	-78.0
Au(24)-S(4)-C(25)-C(26)	50.5
Au(24)-S(14)-C(105)-C(106)	-173.9
Au(25)-S(11)-C(81)-C(82)	-175.1
Au(25)-S(16)-C(121)-C(122)	38.5
Au(26)-S(15)-C(113)-C(114)	93.1
Au(26)-S(16)-C(121)-C(122)	-103.6
S(1)-C(1)-C(2)-C(3)	168.0
S(2)-C(9)-C(10)-C(11)	-128.8
S(3)-C(17)-C(18)-C(19)	179.8
S(4)-C(25)-C(26)-C(27)	173.7
S(5)-C(33)-C(34)-C(35)	-138.4
S(6)-C(41)-C(42)-C(43)	116.2

S(7)-C(49)-C(50)-C(51)	133.8
S(8)-C(57)-C(58)-C(59)	-166.6
S(9)-C(65)-C(66)-C(67)	174.3
S(10)-C(73)-C(74)-C(75)	176.1
S(11)-C(81)-C(82)-C(83)	179.0
S(12)-C(89)-C(90)-C(91)	-161.0
S(14)-C(105)-C(106)-C(107)	149.0
S(15)-C(113)-C(114)-C(115)	152.2
S(16)-C(121)-C(122)-C(123)	91.7
C(1)-C(2)-C(3)-C(8)	76.1
C(1)-C(2)-C(3)-C(4)	-96.6
C(2)-C(3)-C(8)-C(7)	-173.2
C(2)-C(3)-C(4)-C(5)	172.2
C(3)-C(8)-C(7)-C(6)	0.0
C(8)-C(3)-C(4)-C(5)	0.0
C(8)-C(7)-C(6)-C(5)	0.0
C(7)-C(6)-C(5)-C(4)	0.0
C(6)-C(5)-C(4)-C(3)	0.0
C(4)-C(3)-C(8)-C(7)	0.0
C(9)-C(10)-C(11)-C(12)	-132.5
C(9)-C(10)-C(11)-C(16)	45.5
C(12)-C(13)-C(14)-C(15)	0.0
C(13)-C(12)-C(11)-C(10)	177.9
C(13)-C(12)-C(11)-C(16)	0.0
C(13)-C(14)-C(15)-C(16)	0.0
C(14)-C(15)-C(16)-C(11)	0.0
C(15)-C(16)-C(11)-C(10)	-177.9
C(15)-C(16)-C(11)-C(12)	0.0
C(11)-C(12)-C(13)-C(14)	0.0
C(17)-C(18)-C(19)-C(20)	-105.5
C(17)-C(18)-C(19)-C(24)	80.4
C(18)-C(19)-C(20)-C(21)	-174.0
C(18)-C(19)-C(24)-C(23)	174.3
C(19)-C(20)-C(21)-C(22)	0.0
C(20)-C(19)-C(24)-C(23)	0.0
C(20)-C(21)-C(22)-C(23)	0.0
C(21)-C(22)-C(23)-C(24)	0.0
C(22)-C(23)-C(24)-C(19)	0.0

C(24)-C(19)-C(20)-C(21)	0.0
C(25)-C(26)-C(27)-C(32)	123.2
C(25)-C(26)-C(27)-C(28)	-67.4
C(26)-C(27)-C(32)-C(31)	171.2
C(26)-C(27)-C(28)-C(29)	-168.2
C(27)-C(32)-C(31)-C(30)	0.0
C(32)-C(27)-C(28)-C(29)	0.0
C(32)-C(31)-C(30)-C(29)	0.0
C(31)-C(30)-C(29)-C(28)	0.0
C(30)-C(29)-C(28)-C(27)	0.0
C(28)-C(27)-C(32)-C(31)	0.0
C(33)-C(34)-C(35)-C(40)	-74.9
C(33)-C(34)-C(35)-C(36)	102.6
C(34)-C(35)-C(40)-C(39)	177.3
C(34)-C(35)-C(36)-C(37)	-177.8
C(35)-C(40)-C(39)-C(38)	0.0
C(40)-C(35)-C(36)-C(37)	0.0
C(40)-C(39)-C(38)-C(37)	0.0
C(39)-C(38)-C(37)-C(36)	0.0
C(38)-C(37)-C(36)-C(35)	0.0
C(36)-C(35)-C(40)-C(39)	0.0
C(41)-C(42)-C(43)-C(48)	-158.7
C(41)-C(42)-C(43)-C(44)	-11.6
C(48)-C(47)-C(46)-C(45)	0.0
C(47)-C(48)-C(43)-C(42)	149.9
C(47)-C(48)-C(43)-C(44)	0.0
C(47)-C(46)-C(45)-C(44)	0.0
C(46)-C(45)-C(44)-C(43)	0.0
C(45)-C(44)-C(43)-C(42)	-142.6
C(45)-C(44)-C(43)-C(48)	0.0
C(43)-C(48)-C(47)-C(46)	0.0
C(49)-C(50)-C(51)-C(52)	54.6
C(49)-C(50)-C(51)-C(56)	-125.9
C(52)-C(53)-C(54)-C(55)	0.0
C(53)-C(52)-C(51)-C(50)	179.5
C(53)-C(52)-C(51)-C(56)	0.0
C(53)-C(54)-C(55)-C(56)	0.0
C(54)-C(55)-C(56)-C(51)	0.0

C(55)-C(56)-C(51)-C(50)	-179.7
C(55)-C(56)-C(51)-C(52)	0.0
C(51)-C(52)-C(53)-C(54)	0.0
C(57)-C(58)-C(59)-C(60)	74.8
C(57)-C(58)-C(59)-C(64)	-104.0
C(58)-C(59)-C(60)-C(61)	-178.8
C(58)-C(59)-C(64)-C(63)	178.8
C(59)-C(60)-C(61)-C(62)	0.0
C(60)-C(59)-C(64)-C(63)	0.0
C(60)-C(61)-C(62)-C(63)	0.0
C(61)-C(62)-C(63)-C(64)	0.0
C(62)-C(63)-C(64)-C(59)	0.0
C(64)-C(59)-C(60)-C(61)	0.0
C(65)-C(66)-C(67)-C(72)	-8.5
C(65)-C(66)-C(67)-C(68)	178.5
C(66)-C(67)-C(72)-C(71)	-173.0
C(66)-C(67)-C(68)-C(69)	172.9
C(67)-C(72)-C(71)-C(70)	0.0
C(72)-C(67)-C(68)-C(69)	0.0
C(72)-C(71)-C(70)-C(69)	0.0
C(71)-C(70)-C(69)-C(68)	0.0
C(70)-C(69)-C(68)-C(67)	0.0
C(68)-C(67)-C(72)-C(71)	0.0
C(73)-C(74)-C(75)-C(76)	109.0
C(73)-C(74)-C(75)-C(80)	-72.6
C(74)-C(75)-C(76)-C(77)	178.4
C(74)-C(75)-C(80)-C(79)	-178.5
C(75)-C(76)-C(77)-C(78)	0.0
C(76)-C(75)-C(80)-C(79)	0.0
C(76)-C(77)-C(78)-C(79)	0.0
C(77)-C(78)-C(79)-C(80)	0.0
C(78)-C(79)-C(80)-C(75)	0.0
C(80)-C(75)-C(76)-C(77)	0.0
C(81)-C(82)-C(83)-C(88)	109.7
C(81)-C(82)-C(83)-C(84)	-73.5
C(82)-C(83)-C(88)-C(87)	176.9
C(82)-C(83)-C(84)-C(85)	-176.9
C(83)-C(88)-C(87)-C(86)	0.0

C(88)-C(83)-C(84)-C(85)	0.0
C(88)-C(87)-C(86)-C(85)	0.0
C(87)-C(86)-C(85)-C(84)	0.0
C(86)-C(85)-C(84)-C(83)	0.0
C(84)-C(83)-C(88)-C(87)	0.0
C(89)-C(90)-C(91)-C(92)	-95.1
C(89)-C(90)-C(91)-C(96)	82.6
C(90)-C(91)-C(92)-C(93)	178.1
C(90)-C(91)-C(96)-C(95)	-177.3
C(91)-C(92)-C(93)-C(94)	0.0
C(92)-C(91)-C(96)-C(95)	0.0
C(92)-C(93)-C(94)-C(95)	0.0
C(93)-C(94)-C(95)-C(96)	0.0
C(94)-C(95)-C(96)-C(91)	0.0
C(96)-C(91)-C(92)-C(93)	0.0
C(97)-C(98)-C(99)-C(100)	-164.1
C(97)-C(98)-C(99)-C(104)	41.4
C(98)-C(99)-C(100)-C(101)	-150.5
C(98)-C(99)-C(104)-C(103)	160.6
C(99)-C(100)-C(101)-C(102)	0.0
C(100)-C(99)-C(104)-C(103)	0.0
C(100)-C(101)-C(102)-C(103)	0.0
C(101)-C(102)-C(103)-C(104)	0.0
C(102)-C(103)-C(104)-C(99)	0.0
C(104)-C(99)-C(100)-C(101)	0.0
C(105)-C(106)-C(107)-C(108)	118.6
C(105)-C(106)-C(107)-C(112)	-38.8
C(106)-C(107)-C(108)-C(109)	-160.6
C(106)-C(107)-C(112)-C(111)	154.6
C(107)-C(108)-C(109)-C(110)	0.0
C(108)-C(107)-C(112)-C(111)	0.0
C(108)-C(109)-C(110)-C(111)	0.0
C(109)-C(110)-C(111)-C(112)	0.0
C(110)-C(111)-C(112)-C(107)	0.0
C(112)-C(107)-C(108)-C(109)	0.0
C(113)-C(114)-C(115)-C(120)	6.3
C(113)-C(114)-C(115)-C(116)	-173.7
C(114)-C(115)-C(120)-C(119)	180.0

C(114)-C(115)-C(116)-C(117)	-180.0
C(115)-C(120)-C(119)-C(118)	0.0
C(120)-C(115)-C(116)-C(117)	0.0
C(120)-C(119)-C(118)-C(117)	0.0
C(119)-C(118)-C(117)-C(116)	0.0
C(118)-C(117)-C(116)-C(115)	0.0
C(116)-C(115)-C(120)-C(119)	0.0
C(121)-C(122)-C(123)-C(128)	32.3
C(121)-C(122)-C(123)-C(124)	-145.2
C(122)-C(123)-C(128)-C(127)	-177.5
C(122)-C(123)-C(124)-C(125)	177.4
C(123)-C(128)-C(127)-C(126)	0.0
C(128)-C(123)-C(124)-C(125)	0.0
C(128)-C(127)-C(126)-C(125)	0.0
C(127)-C(126)-C(125)-C(124)	0.0
C(126)-C(125)-C(124)-C(123)	0.0
C(124)-C(123)-C(128)-C(127)	0.0